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# Application of simulation and machine learning in supply chain management: A synthesis of the literature using the Sim-ML literature classification framework

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## ABSTRACT

Stochastic modeling techniques, such as discrete-event and agent-based simulation, are widely used in supply chain management (SCM) for capturing real-world uncertainties. Over the last decade, data-driven approaches like machine learning (ML) have also gained prominence in SCM, employing methods such as supervised learning (SL), unsupervised learning (UL), and reinforcement learning (RL). As supply chains grow in complexity, hybrid models combining simulation (Sim) and ML are becoming increasingly common, and the field stands to gain from a structured review of this literature. Towards this, we developed the Sim-ML Literature Classification Framework, which includes a hierarchical taxonomy comprising five SC criteria, 22 Sim-ML classes and over 75 Sim-ML subclasses. We applied this framework to synthesize 99 papers, revealing significant diversity in how Sim-ML models are used to address supply chain challenges. Key findings include the recognition of the breadth of study objectives, identifying various forms of model hybridization achieved by combining discrete/continuous simulation techniques with SL, UL, and RL approaches, and the data flow mechanisms such as sequential and feedback methods employed by the simulation and ML elements of the hybrid model. Our findings also identify some gaps in the literature; for example, optimization is rarely incorporated into Sim-ML models. Also, most studies present Sim-ML models for addressing problems in general supply chains, likely due to the lack of access to industrial data. The review also highlights that Industry 4.0 technologies, such as digital twins and blockchain, are underrepresented in current research, as are topics like sustainability and transportation. These gaps suggest significant opportunities for future research. We provide guidelines for practitioners on applying Sim-ML models to manage supply chain drivers, mitigate the impact of disruptions, and integrate emerging technologies. Our review serves as a valuable resource for researchers, practitioners, and students interested in leveraging Sim-ML approaches in SCM.

## 1. Introduction

Supply chain management (SCM) is a key area of research in Operations Research and Management Science (OR/MS). A study analyzing three decades of OR/MS literature highlights SCM as one of the top three most frequently studied areas during the periods 2000–2009 and 2010–2019 (Mustafee & Katsaliaki, 2020). The study also identifies a range of OR/MS techniques applied to SCM, including analytical modeling, optimization methods, Multi-Criteria Decision Making, Data Envelopment Analysis, game theory, and simulation. These techniques have been instrumental in tackling various challenges in supply chain design, procurement, and closed-loop supply chains.

Among these techniques, simulation has become particularly prominent due to its ability to model the inherent uncertainties in supply chains through stochastic representations. The most commonly used simulation techniques in SCM include discrete-event simulation (DES), agent-based simulation (ABS), and system dynamics (SD). DES models the operation of supply chains as a series of discrete events, making it ideal for detailed process analysis (Terzi & Cavalieri, 2004). ABS, in contrast, focuses on the behaviors and interactions of individual agents within the supply chain, effectively capturing the complexity of decentralized decision-making (Clausen et al., 2019). Meanwhile, SD emphasizes feedback loops and time delays within supply chains, providing valuable insights into long-term trends and dynamic behaviors

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(Badakhshan & Bahadori, 2024). Each simulation technique offers unique advantages, making them essential tools for addressing various aspects of SCM challenges (Mustafee et al., 2021).

As supply chains have grown large and complex, hybrid simulation models have been developed that combine the strengths of individual simulation techniques such as DES, ABS, and SD to capture underlying supply chain complexities and tackle the multifaceted challenges inherent in SCM (Mustafee et al., 2017). By integrating these techniques, hybrid models enhance the ability to capture the dynamic interactions between agents, process flows, and systemic feedback loops. This improves the accuracy of simulations and provides deeper insights into complex supply chains, leading to more effective decision-making. According to Brailsford et al. (2019), SCM is one of the three primary application areas where hybrid simulation has made a significant impact, highlighting the efficacy of the method in advancing supply chain modeling.

Parallel to the advancements in simulation, the last decade has witnessed substantial growth in the application of machine learning (ML) in SCM (Cioffi et al., 2020; Kang et al., 2023). This surge in research has been driven by advances in computational power and the development of algorithms capable of processing and analyzing extensive volumes of complex data. ML offers powerful techniques for uncovering patterns in large datasets, which enable various forms of analytics, e.g., predictive and prescriptive, and decision support. Key applications include demand forecasting (Zhu et al., 2021), supplier selection (Nafei et al., 2024), and disruption management (Brintrup et al., 2020). As supply chains become increasingly data-rich, the role of ML in enhancing efficiency, resilience, and decision-making continues to grow, underscoring its transformative potential in the industry.

Distinct from hybrid simulation, the term hybrid modeling is increasingly used in the literature to identify studies that have combined a simulation technique, such as DES, ABS or SD, with methods and techniques from the wider OR/MS or indeed from different disciplines (Mustafee et al., 2018; Tolk et al., 2021). One such technique is ML, which intersects several fields of study, such as data science, applied computing, mathematics, and statistics. In this paper, the term hybrid model refers to the combined application of a simulation model with an ML approach. Numerous studies have developed Sim-ML models, and this paper aims to identify those specifically applied to SCM.

Recently, in the SCM literature, there has been growing interest in developing hybrid models that integrate DES, ABS, and SD simulations with ML approaches such as SL, UL, and RL. This integrated approach promises to combine the strengths of both methodologies, leading to more accurate models, improved decision-making and enhanced predictive capabilities. By embedding ML algorithms within simulation models, researchers and practitioners can dynamically adapt simulations based on real-time data, effectively capturing the complexities and uncertainties of modern supply chains. Additionally, ML algorithms can be trained using data generated by simulation models, especially when empirical data is unavailable or insufficient. This integration represents a strategic shift towards more intelligent, data-driven SCM, significantly improving the ability to anticipate and respond to uncertainties.

Previous reviews in the literature have primarily focused on simulation and ML in SCM as separate domains. While these reviews have provided valuable insights into the individual applications of simulation and ML, they have not extensively explored their integration. The contribution of this literature review lies in its examination of the integration of simulation and ML in SCM. Specifically, this review aims to answer five research questions: (1) What are the main applications of hybrid modeling using simulation and ML in SCM? (2) What are the most common hybrid modeling combinations used in SCM? (3) What are the data flow mechanisms in hybrid models? (4) How does hybrid modeling support the development of digital twin, which is an Industry 4.0 enabler? (5) What is the extent of the adoption of hybrid modeling in addressing industrial use cases? By addressing these questions, the review uncovers gaps in the existing literature and informs both academic

research and practical implementation. Ultimately, it seeks to enhance the understanding of integrated simulation and ML in SCM and offer strategic insights for future research and development in this vital area.

The remainder of the paper is organized as follows: Section 1.1 presents the scope of this review. In Section 1.2, we present a short review of papers on the applications of ML, simulation, and Industry 4.0 technologies in supply chains, identifying existing gaps in the literature and the contribution of this work. Section 2 outlines the literature review methodology, including the keywords and other variables used for the scholarly search, an illustration of the methodology, and an analysis of the underlying dataset in terms of publication year and type of scholarly output (e.g., journal articles, conference papers, book chapters). Section 3 presents a top-level synthesis of the literature based on bibliometric analysis. Section 4 synthesizes the literature on simulation and ML using our Sim-ML literature classification framework. Finally, Section 5 discusses future research directions and summarizes the main contributions of the literature review.

### 1.1. Scope of the literature review

In the literature, we identify five forms of hybrid models based on Mingers and Brocklesby's (1997) definitions of paradigms, methodologies, techniques, and tools (Mustafee et al., 2020). Model Types A, B, and C represent three forms of hybrid simulation, e.g., DES-ABS, DES-SD, and DES-ABS-SD, and Model Types D and E represent hybrid models that combine simulation with methods and techniques developed outside the M&S field. The reader is referred to Mustafee and Fakhimi (2024) for the taxonomy of hybrid models.

The scope of this paper is on models that combine simulation with ML (this is Model Type D). Thus, the subsequent usage of the term "hybrid model" or "hybrid modeling" will refer to those subtypes of Model Type D that combine simulation techniques such as ABS, DES, and SD with various ML approaches, with or without optimization. The hybrid terminologies will also apply to Model Type E. This enables us to include the increasing number of papers using computer science and applied computing approaches with modeling, for example, linking sensors and real-time data feeds that then populate simulation and ML models, e.g., digital twins and real-time simulation (Mustafee et al., 2023). The scope of our literature review is presented in Table 1.

### 1.2. Existing review papers

Table 2 summarises prior literature reviews on the applications of ML, simulation, and Industry 4.0 technologies in supply chains, as well as on supply chain drivers. Existing studies predominantly focus on the applications of either ML (e.g., Kang et al., 2023; Mahraz et al., 2022; Cioffi et al., 2020) or simulation (e.g., Ferreira et al., 2024; Demartini et al., 2022) in supply chain contexts. The novelty of this study lies in its examination of the integration of simulation and ML techniques to manage supply chain drivers. While the integration of simulation and optimization, commonly referred to as simulation-optimization, has been reviewed in the SCM literature, hybrid models combining simulation and ML has not yet been comprehensively explored. Furthermore, previous reviews on Industry 4.0 technologies in supply chains have not emphasized the role of Sim-ML approaches in the context of these technologies. Similarly, existing reviews on supply chain drivers do not highlight the role of Sim-ML approaches in managing these drivers. This review provides a comprehensive perspective on how Sim-ML techniques can enhance the management of supply chain drivers, mitigate the impacts of supply chain disruptions, and support the development of Industry 4.0 technologies.

In this paper, we introduce the Sim-ML literature classification framework for synthesizing the literature on simulation and ML in SCM. Our framework offers six key contributions: First, it systematically identifies the primary applications of Sim-ML modeling, delivering a comprehensive overview of its current implementation while also

**Table 1**

The scope of the literature review with consideration of the definitions of paradigms, methodologies, techniques and tools (Mingers & Brocklesby, 1997).

Terminology	Definitions	Scope of the Literature Review
Paradigm	Paradigms are “very general set of philosophical assumptions that define the nature of possible research and interventions” (Mingers & Brocklesby, 1997).	The review considers only the Hard OR (quantitative) paradigm. However, it is recognised that qualitative/ Soft OR approaches like Qualitative System Dynamics (causal loop diagrams) and Soft Systems Methodology (SSM) may have been used to aid the development of stock and flow SD simulations or in developing the conceptual model for a DES. The review considers both discrete and continuous methodologies for simulation and simulation-based optimization. In addition, the review includes both ML and ML-driven optimization.
Methodologies	Methodologies develop within paradigms and embody the overarching philosophical assumptions.	The review refers to DES, ABS, SD, supervised learning, reinforcement learning (RL), discrete optimization, etc., as techniques that are derived from overarching methodologies like M&S, ML and optimization, which, in turn, have been developed with the Hard OR paradigm.
Techniques	Techniques exist within methodologies.	Examples of tools in scope include <i>Simul8</i> and <i>Witness</i> (tools for DES), <i>KerasRL</i> and <i>pyqlearning</i> libraries for implementing the Reinforcement Learning (RL) technique.
Tools	Tools are artefacts like commercial-off-the-shelf simulation packages, software for optimization and specific ML algorithms.	

highlighting supply chain challenges that are yet to be addressed through Sim-ML modeling. Second, the classification of extant literature through the framework reveals widely employed Sim-ML model combinations and their application context, which could aid in translating mature areas of Sim-ML research to real-world implementation. Third, the framework identifies underexplored combinations of simulation and ML techniques, which could potentially be used for SC modeling; thus, the framework helps guide future research by identifying fertile areas of inquiry. Fourth, the framework identifies data flow mechanisms within Sim-ML models, which are crucial for understanding how information is exchanged between different simulation and ML techniques, and offers future directions for cross-disciplinary M&S-ML research. Fifth, it maps hybrid models to Industry 4.0 enablers, underscoring the role of Sim-ML modeling in developing digitally-enabled supply chains. Finally, the framework assesses the extent of the adoption of Sim-ML modeling in addressing real-world industrial use cases, offering insights into its practical implementation. Together, these contributions demonstrate the framework’s potential to advance both theoretical knowledge and practical applications in the field, providing a clear direction for future research and application.

In the literature, we find several domain-specific literature classification frameworks that have been adopted by multiple studies. For example, the PPMO framework by Mustafee et al. (2021) was first used to provide the synthesis of the literature on distributed supply chain simulation. PPMO is an acronym for profiling (P) research, analyzing problem (P) definition and context of application, capturing data related to model (M) development, and studying outcomes (O). Other studies have since used the PPMO framework; for example, Kar et al. (2024) used the PPMO framework to classify literature on hybrid simulation in healthcare, and Staff and Mustafee (2023) extended PPMO to categorize

**Table 2**

Scope and objective of existing reviews.

Scope of existing reviews	Authors	Study Objective
Review of studies that use ML for SCM	Akbari and Do (2021), Mahraz et al. (2022), Ni et al. (2020), Wenzel et al. (2019)	Review of ML applications in SCM
	Kang et al. (2023), Rai et al. (2021), Breitenbach et al. (2021), Cioffi et al. (2020)	Review of ML applications in manufacturing supply chains
	Hosseinnia Shavaki and Ebrahimi Ghahnavieh (2023)	Review of deep learning applications in SCM
	Rolf et al. (2023)	Review of reinforcement learning applications in SCM
Review of studies that use simulation for SCM	Ferreira et al. (2024)	Review of simulation modeling applications in hospital waste supply chain
	Korder et al. (2024)	Review of simulation modeling applications in supply chains facing disruptions
	Saisridhar et al. (2024)	Reviews of simulation modeling applications in assessing supply chain responsiveness, resilience, and robustness
	Demartini et al. (2022)	Review of simulation approaches in industrial symbiosis
	Mustafee et al. (2021)	Review of distributed simulation applications in supply chains
	Clausen et al. (2019)	Review of agent-based simulation applications in supply chains
	Oliveira et al. (2016)	Review on agent-based simulation for decision-making in supply chains
Review of studies that use simulation–optimization for SCM	Ghasemi et al. (2024)	Review of applications of simulation–optimization for production scheduling in manufacturing supply chains
	Tordeccilla et al. (2021)	Review of applications of simulation–optimization for designing resilient supply chains
	Pourhejazy and Kwon (2016)	Reviews of applications of simulation–optimization for designing supply chains
Review of Industry 4.0 technologies in supply chains	Rojek et al. (2024)	Review of 6G-based SCM within Industry 4.0 paradigm
	Baziyyad et al. (2024)	Review of data-driven technologies within Industry 4.0 for SCM
	Jetty and Afshan (2024)	Review Industry 4.0 implementation in supply chains
Review of Industry 4.0 technologies in a specific supply chain	Huang et al. (2024)	Review of digital twins’ implementation in the food supply chain
	Escribà-Gelonch et al. (2024)	Review of digital twins in agricultural supply chains
	Ülkü et al. (2024)	Review of Industry 4.0 technologies’ Implementation in humanitarian supply chains
Review literature on supply chain driver(s)	Jahani et al. (2024)	Supply chain network design with financial considerations
	Zarei et al. (2023)	Sustainable sourcing in supply chains

(continued on next page)

Table 2 (continued)

Scope of existing reviews	Authors	Study Objective
	Nielsen et al. (2024)	Transportation in supply chains
	Alnahhal et al. (2024)	Inventory management in supply chains

DES studies on managing perishable inventories. As our review relates to simulation, we first considered whether the PPMO literature classification framework, essentially a listing of variables captured from the papers under different categories, could be employed as an overarching scholarly structure for presenting the Sim-ML literature synthesis. However, our review also includes the analysis of methods from the field of ML and hybrid combinations of simulations with ML models. The scope of the paper thus introduced the need for further analysis related to methodologies, for example, whether the simulation techniques employed were continuous or discrete, whether optimization was a part of the study, the specific data flow mechanisms used by the simulation

and ML sub-models, and so on. We thus concluded that a hierarchical literature classification framework was needed for the paper: The Sim-ML framework. We hope our framework will be used to classify future studies integrating simulation and ML, facilitating the systematic categorization and comparison of emerging Sim-ML approaches. By providing a structured framework for evaluating how new research aligns with existing applications and identifying gaps, the Sim-ML literature classification framework supports the advancement of knowledge and ensures that future studies build upon established insights.

2. Literature review methodology

This review synthesizes scholarly work on hybrid modeling that combines simulation and ML within SCM. Given the interdisciplinary nature of the subject, spanning OR, Industrial Engineering, Data Science, and SCM, a semi-systematic review approach was selected. This approach systematically analyzes relevant literature while allowing

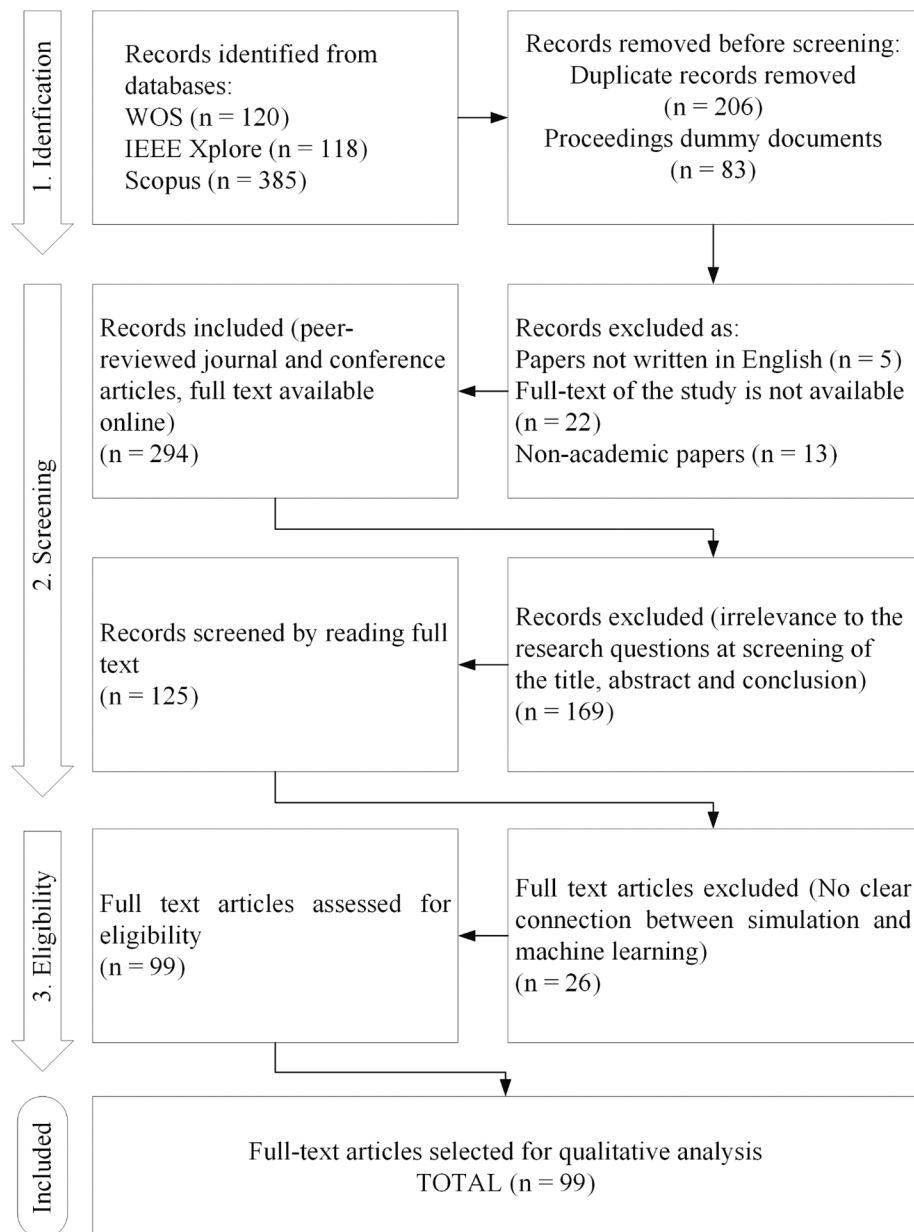


Fig. 1. PRISMA flow diagram.



flexibility in the search and selection process, making it particularly useful for broad or interdisciplinary research fields (Snyder, 2019; Zunder, 2021). The semi-systematic review also helps identify themes conceptualized differently across various fields, thereby establishing an agenda for further research (Wong et al., 2013). We adopted the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) framework to enhance transparency and rigor. This adaptation ensured a structured approach to the literature review process, improving the reproducibility and reliability of our findings (De Felice et al., 2022). Fig. 1 presents the PRISMA flow diagram, summarizing the steps followed for paper selection in this review, which involved three stages: identification, screening, and eligibility. While the identification and screening stages were systematic, the eligibility stage relied on our domain expertise and experience. The following sections detail the steps taken in sequence.

### 2.1. Research questions

The underlying literature for hybrid simulation and ML models comes predominantly from the fields of OR (e.g., simulation and optimization), Data Science (e.g., ML), and Industrial Engineering/Industry 4.0 (e.g., digital twins). Considering this, we formulated the following five research questions (RQs) to guide the development of the search terms.

RQ1: What are the main applications of hybrid modeling using simulation and ML in SCM?

RQ2: What are the most common hybrid modeling combinations used in SCM?

RQ3: What are the data flow mechanisms in hybrid models?

RQ4: How does hybrid modeling support the development of digital twins, which is an Industry 4.0 enabler?

RQ5: What is the extent of the adoption of hybrid modeling in addressing industrial use cases?

### 2.2. Search terms

The search strategy was developed to capture literature on Sim-ML models in SCM, the synthesis of which will help us answer RQs 1–5. To ensure a comprehensive and rigorous exploration of the literature, we adopted a structured approach involving the definition of precise search terms, the selection of relevant databases, and the systematic collection and analysis of pertinent studies.

We developed the search terms iteratively with contributions from all authors, each bringing expertise in simulation, ML, and SCM. These terms were categorized into four main themes: Simulation, Industry 4.0 Digital Twins, Data-driven Learning, and Supply Chain, each aligned with our RQs to ensure comprehensive coverage of hybrid modeling.

In the simulation category, keywords related to DES, ABS, SD, and Monte Carlo were included as these are the dominant techniques in M&S. These keywords also captured studies employing two or more M&S techniques to develop a hybrid simulation (Brailsford et al., 2019). We agreed that digital twins are a topical area of research and included it under Industry 4.0. Similarly, we assigned keywords relevant to ML to the data-driven learning category. We added Supply chain as a keyword as it was the domain of interest. Table 3 lists the keyword combinations for database search. By mapping the RQs to keyword categories, we ensured that we did not overlook important search terms; we then combined these terms to identify the initial dataset for the review.

### 2.3. Database searching and screening criteria

We conducted searches across three major databases known for their extensive coverage of peer-reviewed literature in fields pertinent to our research focus: *ISI Web of Science (WOS)*, *Scopus*, and *IEEE Xplore*. We selected *WOS* for its multidisciplinary reach and emphasis on high-quality research in OR and Industrial Engineering. We included *Scopus*

**Table 3**  
Examples of keyword sets for database search.

Keyword Category	Mapping with RQ	Example keyword combination for search terms	Retrieve papers containing
Simulation	RQ1-RQ5	“discrete-event” OR “discrete event”; agent-based AND (model* OR simul*); “system dynamic*”; Monte-Carlo	Discrete-event simulation, Agent-based modeling, Agent-based simulation, System dynamics, Monte Carlo, Hybrid simulation (as they include a mix of techniques above)
Industry 4.0 Digital Twin	RQ4	Digital twin*;	Digital twin, digital twinning
Data-driven Learning	RQ1-RQ5	“machine learning”; *supervised AND learn*; reinforce* AND learn*	Machine Learning, Supervised ML, Unsupervised ML, Reinforcement Learning
Domain	RQ1, RQ2, RQ5	Supply chain*	Supply chain, supply chain management

for its broad coverage of peer-reviewed literature in science, technology, and engineering; *IEEE Xplore* for its specialist archives on engineering, computer science, and technology research, which are critical for advancements in data science and ML within Industry 4.0. We recognize that a subset of the papers would be retrievable from multiple sites; however, using multiple databases ensured that relevant papers were not missed. The initial search across these databases yielded 623 publications, with Scopus, WOS, and IEEE Xplore contributing to 385, 120, and 118 papers, respectively. Following the initial search, we applied a series of inclusion and exclusion criteria to refine our dataset and concentrate on the most relevant and high-quality research. These criteria are summarized in Table 4.

### 2.4. Screening and quality assessment process

We started with 334 articles after removing duplicates and dummy documents from proceedings. During the screening process, we excluded grey literature, such as reports and other non-peer-reviewed sources, and articles not in English or papers without full-text. This reduced the number of articles to 294. Next, we assessed the titles, abstracts, and conclusions of these 294 papers to determine their relevance to the research questions. Through this process, 169 papers were deemed out of scope. The remaining 125 papers underwent a full-text review, where we independently evaluated each paper for relevance and methodological rigor. To be included, studies needed to directly address the

**Table 4**  
Inclusion and Exclusion Criteria.

Criteria	Inclusion Criteria	Exclusion Criteria
Duplicates	–	Duplicate documents
Proceedings dummy documents	–	Documents categorized as conference reviews that were empty and had no listed authors
Language	Written in English	Non-English papers
Publication Type	Studies published in peer-reviewed journals or conferences	Grey literature (e.g., theses, reports)
Document Availability	Studies available in full-text	Papers without full text
Relevance to research questions	Relevant to our research questions	Irrelevant to research questions
Content Focus	Studies that integrate simulation techniques with ML within the context of SCM	Studies that do not involve the integration of simulation techniques and ML and/or papers that were not on SCM.

integration of simulation and ML within SCM and demonstrate rigorous methodological practices. After this thorough review, we excluded 26 papers because at least two authors agreed that these papers did not provide a clear connection between simulation and ML models, ultimately selecting 99 papers for critical analysis.

Fig. 1 presents the PRISMA flow diagram, outlining the multistage approach we used to select the documents for analysis.

2.5. Document types and annual publication trend

The dataset for the review includes 49 journal articles, 49 conference papers, and one book chapter. Fig. 2 illustrates the annual distribution of publications using a stacked histogram. Between 2000 and 2017, there was no observable trend in publication. However, from 2017, we observed a significant rise; this is not surprising considering the shift from conventional to hybrid simulation over the last decade (Bastani et al., 2022). Further, supply chains are one of the main application areas of hybrid simulation (Brailsford et al., 2019), and the pandemic resulted in demand uncertainty and an increased need to address SC challenges, such as inventory planning and production scheduling, in response to demand surges and declines. This may explain the increase in the literature between 2021 and part of 2023.

3. Analysis of disciplinary research intersects and synthesis of key topics

We conducted two forms of analysis. First, we used WOS and Scopus meta-data to identify the disciplines contributing to the base literature. The subject areas analysis revealed that Computer Science accounts for the largest share, representing 40 % of the articles in the dataset, followed by ORMS (29 %) and Engineering (23 %). Other subject areas, such as Environmental Science, Biochemistry, and Physics, collectively constitute 8 % of the articles (Fig. 3). The prevalence of Computer Science in hybrid modeling literature is not surprising since the field develops novel computational solutions, algorithms, and software essential for implementing complex hybrid models addressing SC problems. Engineering plays a significant role in this literature due to its requirement for modeling intricate, dynamic systems across various application domains, where hybrid models offer versatile and effective representation and analysis. The share of articles in ORMS evidences the applicability of quantitative models using hybrid approaches in addressing complex SC problems.

For the second analysis on synthesizing key topics, we employed VOSviewer (Van Eck & Waltman, 2010) to comprehensively examine the bibliometric network of keywords in the final dataset of 99 papers. Only

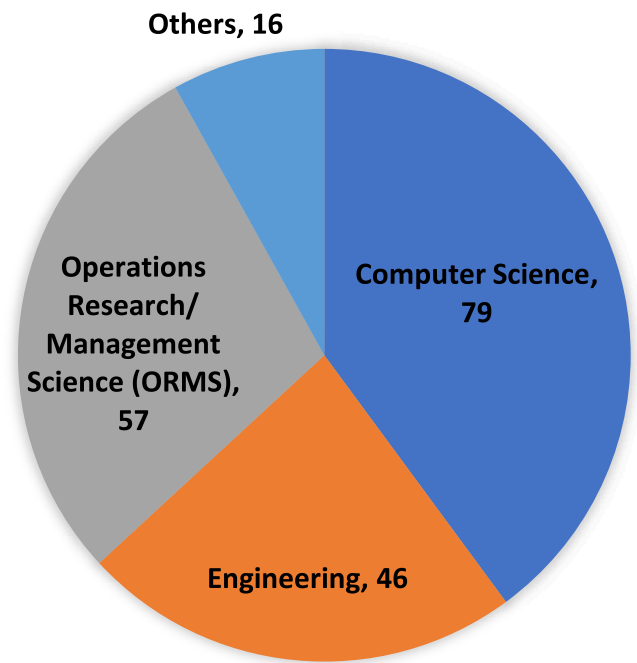


Fig. 3. Subject areas of the publications (papers can appear in more than one category).

keywords that appeared in at least five documents were considered, resulting in 37 keywords meeting this threshold out of a total of 841 keywords. The analysis aims to identify the keywords' relationships and dominant clusters.

Fig. 4 illustrates the bibliometric network featuring the 37 keywords and their associations with co-occurring keywords. The diameter of each circle in the network corresponds to the frequency of occurrences for each keyword. As is to be expected, the keywords identifying our search terms, namely, 'Supply Chains', 'Machine Learning', and 'Reinforcement Learning', are identified as among the most frequently used terms in the VOSviewer analysis.

Furthermore, the visualization of the network highlights two clusters, depicted in green and blue. The analysis of the keywords within the clusters shows that the green cluster is dominated by Industry 4.0 technologies and enablers, such as digital twin and machine learning, and SC concepts, such as inventory management. The red cluster is predominantly associated with decision-making techniques (e.g.,

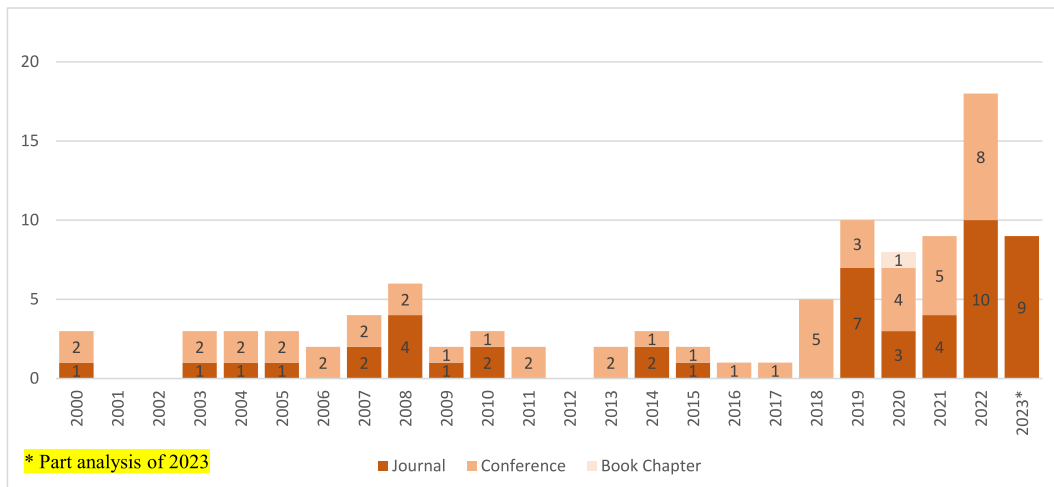


Fig. 2. Number of publications per year (n = 99).

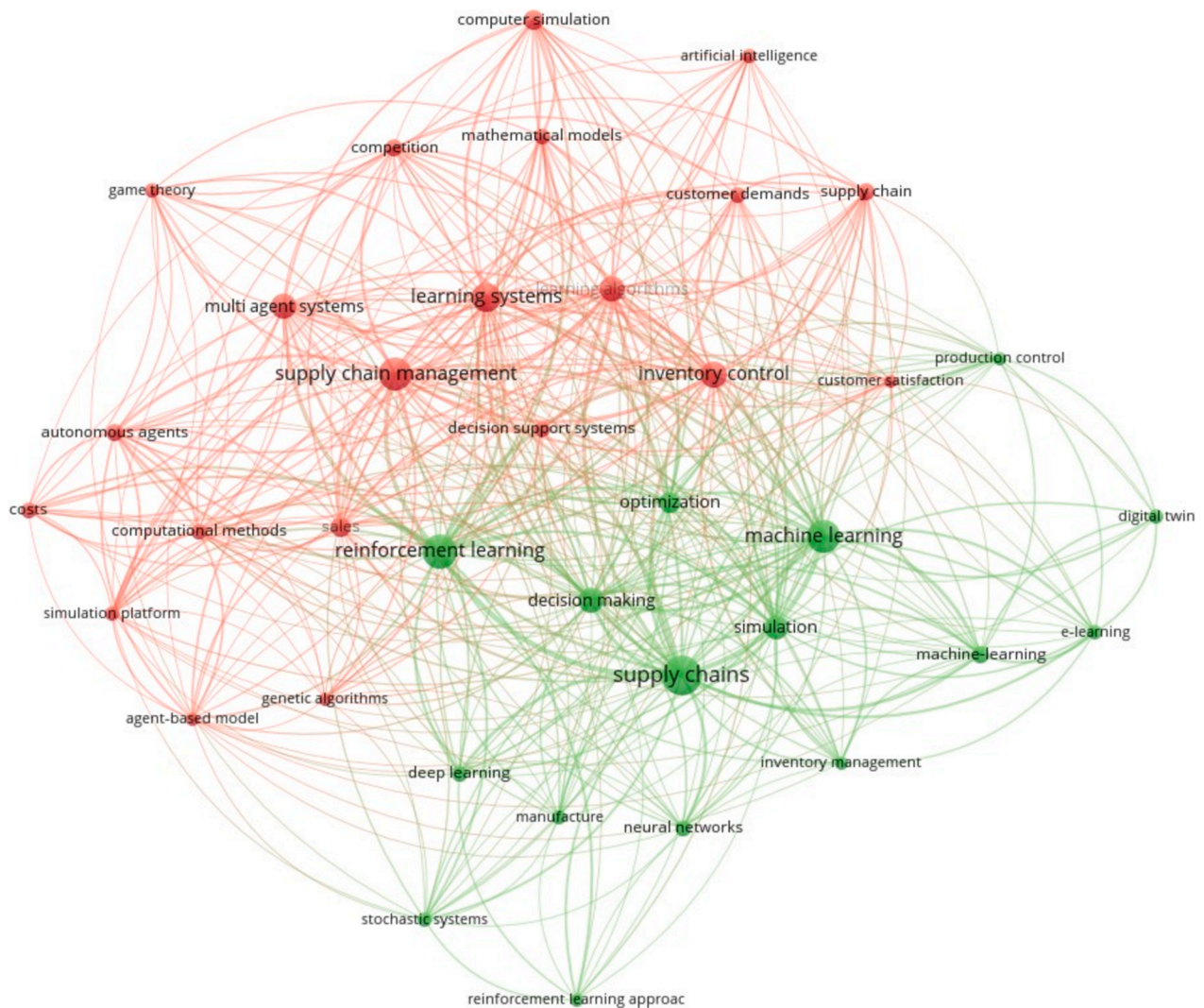


Fig. 4. Bibliometric network of keywords (n = 37).

mathematical models and computer simulation) and application areas such as sales. Considering the broad application of OR methods such as simulation, agent-based modeling, and mathematical modeling in the industry, it is hardly surprising that these methods co-exist in the cluster with keywords related to applications. Compared to the traditional OR methods, data-driven techniques such as machine learning, deep learning, and reinforcement learning (identified by the green cluster) are comparatively more recent. This analysis has not specifically identified hybrid modeling as a keyword. However, as hybrid models employ multiple methods, the keywords are often defined in terms of the specific methods (nearly half of the 37 keywords identified in the VOSviewer analysis relate to specific or associated modeling terms).

To synthesize the literature around the key topics, we decided to employ the method proposed by Ivanov et al. (2021) and Rolf et al. (2023). We organized the keywords into the following two primary clusters based on the analysis of the bibliometric network:

1. SC drivers, data-driven learning, and Industry 4.0 enablers (depicted in green)

(a) SC drivers (e.g., inventory management, production control).

(b) Data-driven learning (e.g., machine learning, deep learning, reinforcement learning).

(c) Industry 4.0 enablers (e.g., digital twin).

2. Modelling methods and applications (depicted in red)

(a) Modelling Methods (e.g., computer simulation, computational

methods, multi-agent systems, mathematical models).

(b) Applications (e.g., sales, costs).

We used the broad categorization of keywords in our primary clusters to guide the subsequent literature analysis, extending relevant existing frameworks and incorporating new categories when necessary, all of which contributed to developing our hierarchical literature classification framework for hybrid studies using simulation and machine learning (Sim-ML).

#### 4. The Sim-ML framework for the synthesis of the literature on simulation and machine learning

As mentioned in the introduction (Section 1.1), the scope of this paper, and by extension the Sim-ML framework presented in this section, is on models that combine simulation with ML (this is a Model Type D) and which may additionally use real-time data feeds by integrating such models with technological artifacts, approaches and standards developed in disciplines such as applied computing and information systems (Type E model). We employ a framework-based approach to classify literature on the aforementioned hybrid model types. The proposed framework is called the Simulation (Sim)-Machine Learning (ML) framework, or Sim-ML for short. It is a hierarchical classification framework consisting of three levels: criteria, classes, and subclasses. We adopted a methodological approach to identify the Sim-ML criteria,



classes, and subclasses, and the resultant Sim-ML classification framework enabled us to present a comprehensive analysis of hybrid models utilized in SCM. Our approach to developing the classification framework is described next.

**Criteria:** The examination of published works revealed significant variations in hybrid models employed to address SC problems, including differences in objectives, modeling techniques, algorithms, Industry 4.0 technologies (the enablers), and industrial use cases. From these variations, we established five criteria that can be organized within a classification framework to help address the research questions (RQs; refer to section 2.1). The five criteria and a short description of each criterion and its mapping with RQs are presented below.

**SC Drivers** – Captures the objectives of the models. They influence SC performance and serve as optimization targets (mapped to RQ1).

**Modeling Techniques and Algorithms** – Evaluate the Sim-ML hybrid models from the perspective of simulation techniques and ML algorithms and approaches (RQ2).

**Data Flow Mechanisms** – Identifies data exchange approaches in hybrid models (RQ3).

**Industry 4.0 Support Technologies** – Informs the role of hybrid modeling in supporting the development of Industry 4.0 digital twin (RQ4).

**Industrial Sectors** – Presents the classification of industrial sectors, which helps to understand the extent of hybrid modeling implementation in real-world SCs (RQ5).

**Classes and Subclasses:** The classes and sub-classes of the Sim-ML framework have been either derived from existing literature or introduced by us when further categorization was needed. For literature-based identification, we extended the supply chain (SC) decision-making framework by [Chopra and Meindl \(2013\)](#) to derive the classes for the Sim-ML criteria of SC drivers. The classes and sub-classes for industrial sectors were informed by the *International Standard Industrial Classification (ISIC)* ([UNO 2008](#)). Finally, we introduced literature-informed classes and sub-classes for the Sim-ML criteria of modeling techniques; this extended the hybrid modeling and simulation classification presented by [Mustafee et al. \(2020\)](#). Only sub-classes with at least one assigned publication were included.

The Sim-ML Literature Classification Framework is presented in [Table 5](#). It comprises a hierarchical classification of five Sim-ML Criteria (column 1), divided into 22 Sim-ML Classes (column 2), and further divided into approx. 75 Sim-ML Subclasses (column 3). The framework’s building blocks (Criterion, Class, and Subclass) are discussed in the following sections with reference to the extant literature.

4.1. Sim-ML Criterion: SC drivers

Each SC strives to maximize the overall value generated, which is the final product’s value minus the incurred SC costs. Achieving this objective involves a complex interplay of various interconnected SC drivers, such as production and logistics, that collectively influence the overall value. Hybrid modeling in SCM is commonly employed to tackle optimization problems by adjusting one or more drivers to enhance SC performance ([Kaur and Singh, 2021](#)). However, accommodating all drivers in a single model is impractical. Therefore, most publications focus on well-defined SC optimization problems, targeting specific drivers. [Chopra and Meindl \(2013\)](#) identify six key drivers that significantly impact supply chain performance: facilities, inventory, transportation, information, sourcing, and pricing. While [Chopra and Meindl’s \(2013\)](#) framework has been foundational in SCM, it omits sustainability, which has become an essential driver in modern SCM. Our literature classification framework builds upon this foundation by introducing a seventh driver: sustainability. This addition emphasizes the importance of incorporating environmental and social considerations into SCM. By integrating sustainability, we aim to assess the extent of hybrid models’ application for improving environmental and social sustainability within supply chains.

**Table 5**

Overview of the Sim-ML Literature Classification Framework with section numbers for Sim-ML Criteria and Sim-ML Classes (Sim-ML Subclasses are in the same sub-section as their corresponding Sim-ML Classes).

Sim-ML Criterion	Sim-ML Class (sub-section number)	Sim-ML Subclass
SC Drivers (Section 4.1)	Facility (4.1.1)	Collaborative SC configuration; Non-collaborative SC configuration
	Inventory (4.1.2)	Customer-managed inventory; Vendor-managed inventory; Production planning; Production scheduling; Working capital management
	Transportation (4.1.3)	Vehicle routing
	Information (4.1.4)	Forecasting; Risk management; Supply Chain Collaboration
	Sourcing (4.1.5)	Supplier selection
	Pricing (4.1.6)	Dynamic pricing; Reverse auction
	Sustainability (4.1.7)	Energy consumption planning; Carbon emission auction; Investment; Circular economy
Modeling Techniques and Algorithms (Section 4.2)	Discrete Simulation Methods with ML (4.2.1)	DES-SL; DES-UL; DES-RL; ABS-SL; ABS-RL
	Acronyms used for sub-classes: DES-discrete-event simulation, ABS-agent-based simulation, SD-system dynamics, MCS-Monte Carlo simulation, SL – supervised learning, UL – unsupervised learning; RL – reinforcement learning, OPT – optimization, SM – simulation model	DES-SL-OPT; ABS-RL-OPT
	Continuous Simulation Methods with ML (4.2.2)	SD-SL
	Continuous Simulation Methods with ML and Optimization (4.2.2)	SD-SL-OPT
	Monte Carlo Methods with ML (4.2.3)	MCS-SL; MCS-RL
	Monte Carlo Methods with ML and Optimization (4.2.3)	MCS-UL-OPT
	Hybrid Simulation with ML (4.2.4)	DES-SD-SL; DES-SD-UL; DES-MCS-RL; SD-ABS-RL; ABS-MCS-SL; DES-SD-ABS-RL
	Hybrid Simulation with ML and Optimization (4.2.4)	DES-SD-SL-OPT; DES-ABS-SL-OPT
	Simulation Model (SM)* with ML (4.2.5)	SM-SL; SM-RL
	Simulation Model (SM)* with ML and Optimization (4.2.5)	SM-SL-OPT; SM-UL-OPT; SM-RL-OPT
Data Flow (DF) Mechanisms (Section 4.3)	Hybrid ML with Discrete Simulation Methods (4.2.6)	SL-DES-RL; DES-ABS-UL-SL
	Sequential Data Flow (4.3.1)	ML followed by simulation (DF Type A); Simulation followed by ML (DF Type B)
	Feedback Data Flow (4.3.2)	ML followed by simulation-based optimization (SBO) (DF Type C)SBO followed by ML (DF Type D) Simulation followed by ML followed by optimization (DF Type E) ML followed by simulation followed by optimization (DF Type F) Reinforcement learning coupled with simulation

(continued on next page)

Table 5 (continued)

Sim-ML Criterion	Sim-ML Class (sub-section number)	Sim-ML Subclass
		(DF Type G)Reinforcement learning coupled with simulation and heuristics (DF Type H)
	Sequential-feedback Data Flow (4.3.3)	Reinforcement learning followed by optimization (DF Type I)Optimization followed by training an RL model using simulation data (DF Type J)
Industry 4.0 Tech. (Section 4.4)	Support Technologies (4.4.1)	Digital Model; Digital Shadow; Digital Twin; Blockchain; Cloud manufacturing
Industrial Sectors (Section 4.5)	Manufacturing (4.5.1)	Electrical equipment; Basic metals; Transport equipment; Machinery and equipment; Computer, electronic, & optical products; Food products; Pharmaceuticals, medicinal chemicals, & botanical products; Coke & refined petroleum products; Motor vehicles, trailers & semi-trailers; Fabricated metal products; Other manufacturing
	Transportation and Storage (4.5.2)	Postal and courier activities
	Electricity, gas, steam, & air conditioning (4.5.3)	Manufacture of gas; Distribution of gaseous fuels through mains
	Wholesale and retail trade (4.5.4)	Retail trade
	Human health and social work activities (4.5.5)	Human health activities

Note (Table 5): \* The term simulation model (SM) is used in this subclass without specifying the applied simulation technique, as the authors have not explicitly mentioned the technique.

This section develops a classification framework based on these seven drivers. Full-text reading of the papers in our dataset enables us to map publications to specific drivers and helps us derive classes and subclasses. Most publications implement hybrid models and present quantitative results, facilitating their assignment to a specific SC driver based on input variables and performance metrics. In rare cases where a publication addresses multiple SC drivers, it is assigned to more than one driver.

#### 4.1.1. Sim-ML Class: Facility

In the context of SC management, a facility refers to a physical location or a place where various activities related to the production, storage, and distribution of goods or services occur. Facilities play a crucial role in the SC as they serve as nodes where products are manufactured, processed, stored, and shipped to meet customer demands (Nobil et al., 2018). Facilities can include manufacturing plants, warehouses, distribution centers, retail stores, and even transportation hubs such as ports and airports. Each facility in the SC network serves a specific purpose, and their effective management is essential to ensure a smooth and efficient flow of goods through the SC (Melo et al., 2009). The SC configuration problem aims to select SC facilities to meet customers' demands while minimizing the overall cost. Optimization is the prevalent technique for tackling the SC configuration problem. To accommodate SC dynamics, optimization models conduct scenario analysis, evaluating various scenarios with different parameters or assumptions to gauge SC responses under different conditions. However, running numerous scenarios can significantly increase computational

time.

On the other hand, hybrid models have the potential to consider multiple scenarios without sacrificing computational efficiency. This advantage stems from combining the strengths of various modeling techniques, including simulation, optimization, and ML. We have identified two subclasses of the facility driver that primarily differ in information exchange (Table 6).

In the remainder of the paper, the < Class>: <Subclass > notation may be used when referring to subclasses. As the Sim-ML classification is hierarchical, prefixing the top-level element (class) to the subclass provides additional context regarding classification hierarchy.

**Facility: Collaborative SC** configuration involves the sharing of information among SC members during the configuration of the SC network. For example, Dahlem and Harrison (2010) utilized hybrid modeling to collaboratively configure an SC network, demonstrating that this approach improved performance metrics such as reduced waiting times and enhanced resource utilization.

**Facility: Non-collaborative SC configuration** is exemplified in studies by Jacobson et al. (2021) and Emerson and Piramuthu (2004). Both studies addressed the SC configuration problem without information sharing among SC members. In these cases, every SC member independently selected their partners without shared knowledge. Nonetheless, both studies highlighted the benefits of hybrid modeling, emphasizing its ability to enhance computational efficiency and improve overall SC performance.

#### 4.1.2. Sim-ML Class: Inventory

Inventory refers to the stock of raw materials, work in process, and finished goods at different stages of the supply chain (Felea, 2008). Inventory management is a widely studied optimization problem in SCM that revolves around determining when and how much to order or produce to balance material availability and inventory costs. Traditional inventory models make simplifying assumptions such as constant demand, lead times, ordering cost, and holding cost. These assumptions may not reflect the dynamics of real-world SCs. Hybrid models can adapt to varying demand patterns, changing lead times, and fluctuating costs more effectively than traditional models with fixed parameters. This adaptability allows SC members to respond to changes in the environment. The inventory driver of the framework encompasses all publications focused on establishing quantities and timing for orders as well as quantities and timing for production. Table 7 lists the subclasses for the inventory driver, followed by a discussion based on the literature.

**Inventory: Customer-managed inventory** refers to managing and controlling inventory by the customer rather than the supplier. In customer-managed inventory, the customer monitors product usage, sets reorder points, and manages replenishment orders. This approach is often used when customers have highly variable or unpredictable demand patterns. For instance, Raghuram et al. (2022) applied hybrid modeling to identify a biomedical equipment manufacturer's optimal safety stock inventory in the presence of demand and supply uncertainty. Priore et al. (2019) employed hybrid modeling to dynamically select replenishment policies that minimize the bullwhip effect in SCs.

**Inventory: Vendor-managed inventory (VMI)** includes a supplier or vendor responsible for monitoring and managing the inventory levels of their products at a customer's location. In VMI, the supplier, rather

Table 6  
Subclasses of the Sim-ML class: facility.

Sim-ML Subclass	Description	Publications
Collaborative SC configuration	Determine the optimal structure of SC to minimize waiting time and maximize utilization.	Dahlem and Harrison (2010)
Non-collaborative SC configuration	Select SC partners using the available knowledge.	Emerson and Piramuthu (2004), Jacobson et al. (2021)

**Table 7**  
Subclasses of the inventory driver.

Sim-ML Subclass	Description	Publications
Customer-managed inventory	The customer monitors inventory levels, sets reorder points, and places replenishment orders to suppliers.	Raghuram et al. (2022), Wang et al. (2022), Priore et al. (2019), Jinqi et al. (2017), Mortazavi et al. (2015), Saitoh and Utani (2013), Kim et al. (2010), Jiang and Sheng (2009), Pan (2008), Zhang and Bhattacharyya (2007), Sheremetov et al. (2005), Ravulapati et al. (2004), Rao et al. (2003), Okada et al. (2023), Guo et al. (2023), Sankaran et al. (2022), Kosasih and Brintrup (2022), Corsini et al. (2022), El Shar et al. (2022), Jackson et al. (2021), Clark and Kulkarni (2021), Barat et al. (2019a), Zhou and Zhou (2019), Barat et al. (2019b), Zhou et al. (2015), Mehta and Yamparala (2014), Ktenioudaki et al. (2021), Zhang et al. (2013), Sheremetov and Rocha-Mier (2008), Kurian et al. (2023), Badakhshan and Ball (2023)
Vendor-managed inventory	The supplier is responsible for monitoring and managing the inventory levels of their products at customer locations.	Afridi et al. (2020), Yang et al. (2015), Sui et al. (2010), Kwon et al. (2008), Chi et al. (2007), Li et al. (2008), Lin and Pai (2000), Xu et al. (2009), Kim et al. (2005)
Production planning	The production planning function determines the types and quantities of goods to produce.	Karimi-Mamaghan et al. (2020), Lee and Sikora (2019), Behnamfar et al. (2022), Weihrauch et al. (2018), Sheremetov et al. (2005), Creighton and Nahavandi (2002), Tuncel et al. (2014), Cao (2003), Lin and Pai (2000), Badakhshan and Ball (2024)*
Production scheduling	The production scheduling function identifies a detailed plan or schedule that outlines the specific production activities and timelines for producing goods.	*Note: Badakhshan and Ball (2024) was first made available online in 2023 and is considered in our analysis of publications (Fig. 2) for that year. Liebenberg and Jarke (2023), Serrano-Ruiz et al. (2022), Lang et al. (2020), Idrees et al. (2006), Zhang et al. (2018), Waschneck et al. (2018), Gros et al. (2020), Greis et al. (2022), Serrano-Ruiz et al. (2021)
Working capital management	The driver relates to inventory and cash policies that optimize working capital.	Badakhshan and Ball (2023), Badakhshan et al. (2022)

than the customer, is responsible for ensuring that the right amount of inventory is available to meet demand. This approach is often used when customer demand is relatively stable and can be forecasted accurately. Afridi et al. (2020) applied hybrid modeling to optimize inventory levels for a semiconductor supplier responsible for managing a manufacturer's inventory. In a similar vein, Yang et al. (2015) utilized hybrid modeling to minimize the bullwhip effect in a VMI system by dynamically determining the replenishment quantity. Sui et al. (2010) also employed hybrid modeling to address a VMI, considering uncertainties in demand and holding cost.

**Inventory: Production planning** encompasses the strategic decision-making process of defining the types and quantities of goods to

produce within a specified timeframe to meet demand and minimize costs, all while carefully considering resource constraints such as labor, materials, and machinery. Hybrid modeling techniques offer significant advantages for production planning. They enable the integration of real-time data, such as demand fluctuations and SC disruptions, resulting in more accurate and responsive production plans. Hybrid models can support extensive "what-if" analysis, allowing production planners to evaluate various planning alternatives and make informed decisions. Additionally, as these models use a mix of simulation, optimization, and ML methods, they have the potential to balance conflicting production objectives, such as cost and lead time minimization, while maintaining computational efficiency. Further, such hybrid models can be developed to provide a comprehensive view of the production planning process, aiding in more informed and effective decision-making. Badakhshan and Ball (2024) demonstrated the practical application of hybrid modeling for updating SC production plans in response to demand and lead time disruptions. Weihrauch et al. (2018) developed a conceptual model that leveraged hybrid modeling to identify disruptions and conduct scenario analysis in semiconductor SCs. Karimi-Mamaghan et al. (2020) utilized hybrid modeling techniques to effectively balance the trade-off between minimizing production costs and minimizing production lead times.

**Inventory: Production scheduling** is the process of determining the sequence and timing of production activities to ensure the efficient use of resources and meet the production plan's objectives. It involves allocating tasks and resources to specific machines, workstations, or production lines in a way that optimizes productivity and minimizes downtime (Fuchigami & Rangel, 2018). Hybrid modeling techniques offer several advantages for production scheduling. Firstly, they can integrate real-time data (Type E Model; see Mustafee et al. (2020)), such as machine performance, demand fluctuations, and inventory levels, for more accurate and responsive scheduling. Secondly, hybrid models can adapt to changing production conditions and make real-time adjustments, ensuring schedules remain optimal in dynamic environments. Thirdly, hybrid models enable production schedulers to conduct in-depth "what-if" analysis, allowing them to assess different scheduling options and select the most effective approach. Liebenberg and Jarke (2023) demonstrated how the use of hybrid modeling for production scheduling enables a transition from mass production to mass customization. Serrano-Ruiz et al. (2022) presented a conceptual framework based on hybrid modeling to integrate real-time data and make real-time adjustments to a production schedule in a job shop manufacturing system. Zhang et al. (2018) applied hybrid modeling to perform extensive scenarios and "what-if" analyses in a job shop manufacturing system and make real-time batching decisions.

**Inventory: Working capital management** is the strategic oversight of a company's short-term assets and liabilities to ensure the effective management of day-to-day financial operations. This practice involves the careful monitoring, control, and optimization of a company's current assets and liabilities. The primary objectives are to maintain liquidity, meet short-term financial obligations, and enhance overall profitability. Current assets encompass cash, accounts receivable, and inventory, while current liabilities include accounts payable and short-term debts. A pivotal metric in evaluating a company's working capital efficiency is the Cash Conversion Cycle (CCC), which measures the time it takes to convert inventory investments into cash flow from sales. Badakhshan and Ball (2023) used hybrid modeling to identify the inventory and cash policies that minimize the manufacturer's CCC in a three-echelon SC in the presence of physical and financial disruptions. Badakhshan et al. (2022) applied hybrid modeling to minimize the CCC for SC rather than each SC member.

#### 4.1.3. Sim-ML Class: Transportation

In the context of SCM, transportation refers to the physical movement of products from one location to another. It plays a crucial role in SCM by facilitating the logistics of moving goods from suppliers to manufacturers, then from manufacturers to distributors, and ultimately

to end customers. Transportation employs various modes, including road, rail, air, and sea, depending on the nature of the products and the distance they need to travel. Efficient transportation is essential to ensure timely product delivery, precise destination arrival, and cost-effectiveness, which directly influence overall supply chain performance and customer satisfaction (Crainic & Laporte, 2016).

Hybrid models that combine optimization, simulation, and ML offer a more comprehensive representation of complex SC transportation systems. They excel in terms of solution quality and computational efficiency. These models empower decision-makers with an all-encompassing view of the transportation network, allowing for optimized routes, modes, and scheduling while considering cost, time, and other critical factors. Additionally, hybrid models integrate real-time data, including traffic updates, inventory levels, and demand fluctuations, enabling dynamic adjustments to transportation plans in response to changing conditions. This real-time adaptability enhances responsiveness and overall efficiency. Table 8 lists the four papers in our dataset that have developed hybrid models related to vehicle routing.

**Transportation: Vehicle routing** pertains to the strategic planning and optimization of delivery or transportation routes. It aims to efficiently distribute goods from a central hub or distribution center to various destinations, including customers, retailers, or suppliers. This process involves determining the most cost-effective and time-efficient way to assign deliveries to vehicles, establish the order of stops, and ensure all goods reach their destinations, all while considering factors like vehicle capacity, delivery time windows, traffic conditions, and other constraints. Effective vehicle routing is pivotal in minimizing transportation costs and delivery times.

Studies addressing the last-mile delivery problem, a subset of the broader vehicle routing problem, have increasingly turned to hybrid modeling techniques. Last-mile delivery, the final stage in the transportation process, involves moving goods from a distribution center or transportation hub to the end consumer's location. This phase is often seen as the SC's most critical and cost-intensive part, striving to meet customer expectations for swift, efficient, and convenient delivery. With the surge in e-commerce and online shopping, last-mile delivery has garnered significant attention from retailers and logistics companies. It comes with various challenges, including optimizing delivery routes, tackling urban congestion, and ensuring efficient and dependable delivery methods. Schnieder et al. (2023) addressed a last-mile delivery problem by integrating an ML model for demand forecasting and a simulation model for land efficiency and emissions prediction. Zou et al. (2022) employed hybrid modeling to adjust delivery routes dynamically in the context of last-mile delivery. Zdolsek Draksler et al. (2023) utilized hybrid modeling to provide real-time delivery recommendations within a last-mile delivery system.

4.1.4. Sim-ML Class: Information

Information within the context of SC management encompasses the data and knowledge required for the planning, coordination, and control of various processes. As data forms the basis for decision-making, the information category plays a pivotal role in all aspects of the SC (Wu & Pagell, 2011). In harnessing this information, ML models take center stage, particularly using supervised learning algorithms, which excel when clear input-output pairs are available, as is often the case in forecasting applications (Rolf et al., 2023). Hybrid models, which incorporate ML techniques, are widely adopted to facilitate informed

**Table 8**  
Subclasses of the transportation driver.

Subclass	Description	Publications
Vehicle routing	Determine the optimal delivery route to minimize delivery costs and maximize delivery speed.	Zdolsek Draksler et al. (2023), Gutierrez-Franco et al. (2021), Schnieder et al. (2023), Zou et al. (2022)

decision-making and enhance the efficiency and effectiveness of SC operations. Table 9 lists studies in our database that can be mapped to the information driver.

**Information: Forecasting** is the process of predicting future events, outcomes, or trends based on historical data and patterns. It involves using mathematical, statistical, or ML techniques to analyze past data and identify patterns that can be used to predict future values or behaviors (Feizabadi, 2022). Hybrid models encompassing ML techniques have been used to forecast SC performance. For instance, Roozkhosh et al. (2023) predicted the acceptance rate of blockchain by integrating system dynamics simulation and ML. Pereira and Frazzon (2021) implemented surrogate-based optimization (SBO) by developing a surrogate model that used ML for demand forecasting. Gruzauskas et al. (2019) used ML to forecast demand, which was used as an input into a simulation model for predicting product waste.

**Information: Risk management** refers to the process of identifying, assessing, and mitigating potential risks that can affect the efficiency and effectiveness of SC operations. This includes identifying risks associated with various aspects of the SC, such as procurement, manufacturing, and transportation. Risk management involves both proactive and reactive planning, leading to improved SC resilience.

Hybrid modeling is used for both proactive and reactive planning. In the proactive approach, hybrid models consider various risks, from demand and supply disruptions to geopolitical and environmental factors, and assess their impact on SC performance. Moreover, hybrid models perform scenario analysis to understand how different scenarios affect SC's risk exposure, which helps in developing contingency plans. In reactive planning, hybrid models provide data-driven recommendations for adjusting production, reallocating resources, or rerouting shipments to minimize disruption effects. Yang et al. (2022) used hybrid modeling to study the impact of flooding disruptions on SC performance and develop strategies to minimize recovery time. Jaenichen et al. (2022) and Shayeez and Panicker (2021) used simulation to investigate the impact of COVID-19 disruptions on SC service and inventory levels and used ML to identify strategies for improving SC resilience.

**Information: Supply Chain (SC) Collaboration** is a strategic approach in which different entities within a SC, such as suppliers, manufacturers, distributors, and retailers, work together to achieve and enhance the overall performance of the SC. The main idea behind SC collaboration is to improve coordination, communication, and cooperation among all parties involved in the SC; this reduces costs and increases responsiveness. Hybrid models can integrate data from various

**Table 9**  
Subclasses of the information driver.

Subclass	Description	Publications
Forecasting	Using historical data to predict future events or identify patterns.	Carbonneau et al. (2008), Guo et al. (2023), Pereira and Frazzon (2021), Sishi and Telukdarie (2021), Gruzauskas et al. (2019), Pereira et al. (2018), Mehta and Yamparala (2014)
Risk management	Identifying, assessing, and mitigating the impact of risks on SC performance (Proactive planning). Mitigating the impact of disruptions on SC performance (reactive planning).	Roozkhosh et al. (2023), Li and Zhao (2006), Yang et al. (2022), Mukherjee et al. (2022), Jaenichen et al. (2022), Shayeez and Panicker (2021), Wang et al. (2020), Yang et al. (2019), Aghaie and Hajian Heidary (2019), Ben Kacem et al. (2020), Badakhshan and Ball (2023), Badakhshan and Ball (2024), Xiang (2020)
Supply Chain Collaboration	Collaboration among SC members to reduce cost and increase responsiveness.	Dahlem and Harrison (2010), Bodendorf et al. (2022), Xiang (2020), Kaihara and Fujii (2008)



SC partners that help achieve transparency and visibility across the entire SC, making it easier for partners to collaborate effectively. For instance, [Bodendorf et al. \(2022\)](#) applied hybrid modeling for collaborative cost management in supplier–buyer dyads. [Xiang \(2020\)](#) used hybrid modeling to minimize the recovery time needed after an energy shortage by SC collaboration. [Kaihara and Fujii \(2008\)](#) developed a hybrid model which considered negotiation between SC members.

#### 4.1.5. Sim-ML Class: Sourcing

Sourcing refers to the process of identifying, evaluating, and selecting suppliers of goods and services. It involves procuring and acquiring materials, components, products, or services needed to support SC operations. Sourcing decisions are critical because they impact various aspects of the SC, including cost, quality, and service level. [Table 10](#) shows the only subclass of the sourcing driver.

**Sourcing: Supplier selection** includes studies that focus on choosing suppliers from a pool of potential candidates. Hybrid models allow for the integration of various data sources and modeling techniques, providing a more comprehensive and holistic view of potential suppliers. This can include historical performance data, financial stability indicators, quality metrics, and more. [Cavalcante et al. \(2019\)](#) and [Etemadidavan and Collins \(2022\)](#) presented hybrid models that used delivery reliability data to select suppliers. Supplier selection often involves evaluating suppliers based on multiple criteria, such as cost, quality, lead time, and sustainability. Hybrid models can handle multi-criteria decision-making by assigning weights to each criterion and objectively comparing suppliers. This ensures that no single criterion dominates the selection process.

#### 4.1.6. Sim-ML class: pricing

Pricing denotes the process of determining the cost at which goods or services are bought or sold within the SC. It involves setting prices at various stages of the SC, from the procurement of raw materials to the sale of finished products to end customers. Pricing decisions have a significant impact on the overall profitability and competitiveness of a SC. [Table 11](#) lists the subclasses of the pricing driver and related publications from our dataset (99 articles).

**Pricing: Dynamic pricing** involves adjusting prices based on various factors, including demand, supply, competitor pricing, and customer behavior. Some forms of hybrid models can integrate data from various sources, including historical sales data, customer behavior data, competitor pricing data, and market trends. This comprehensive data integration provides a holistic view of the variables affecting pricing decisions. In their study, [Du and Xiao \(2019\)](#) employed a combination of ABS and RL to identify effective pricing strategies for adaptive retailers in the face of complex consumer behavior. Similarly, [Hirano et al. \(2021\)](#) integrated ABS and RL to mitigate unintentional collusion arising from auto pricing in SC markets.

**Pricing: Reverse auction** is used in procurement processes where multiple suppliers can provide the required goods or services. They are often employed to source items such as raw materials, components, equipment, or transportation services. The primary objective of a reverse auction is to secure the best possible terms for the buyer, which typically includes competitive pricing and favorable terms and conditions. Suppliers can use hybrid models to analyze various bidding strategies, considering factors such as price, lead time, production capabilities, and market demand. Hybrid models can simultaneously consider a wide range of variables to help suppliers determine the most

**Table 10**  
Subclasses of the sourcing driver.

Subclass	Description	Publications
Supplier selection	Select suppliers from a pool of potential candidates.	<a href="#">Cavalcante et al. (2019)</a> , <a href="#">Etemadidavan and Collins (2022)</a> , <a href="#">Lei et al. (2000a)</a> , <a href="#">Lei et al. (2000b)</a> , <a href="#">Lee and Sikora (2019)</a>

**Table 11**  
Subclasses of the pricing driver.

Subclass	Description	Publications
Dynamic pricing	Updating prices in response to demand, supply, competitor pricing, and customer behavior.	<a href="#">Du and Xiao (2019)</a> , <a href="#">Rana and Oliveira (2014)</a> , <a href="#">Hirano et al. (2021)</a> , <a href="#">Liu et al. (2011)</a> , <a href="#">Kiekintveld et al. (2007)</a> , <a href="#">Pardoe and Stone (2007)</a>
Reverse auction	Determining the bidding price by considering the price, lead time, production capabilities, market demand, and other factors.	<a href="#">Pardoe and Stone (2005)</a> , <a href="#">Pardoe and Stone (2004)</a>

competitive and profitable bidding strategy. [Pardoe et al. \(2004\)](#) and [Pardoe and Stone \(2004\)](#) utilized data generated by ABS models to train decision tree models for determining the bidding price of a supplier in an electronic commerce supply chain.

#### 4.1.7. Sim-ML Class: sustainability

Sustainability in the SC refers to managing SC operations in an environmentally, socially, and economically responsible way. It involves considering the long-term impacts of SC decisions on the environment, society, and the financial stability of the companies involved (also referred to as the triple bottom line of sustainability). Sustainable SCM focuses on minimizing the negative effects while maximizing positive contributions to these areas. [Table 12](#) presents the four subclasses of the sustainability driver that have been identified in our Sim-ML framework for literature synthesis.

**Sustainability: Energy consumption planning** in SC involves strategies and actions to optimize and manage energy use throughout the SC. It aims to reduce energy consumption, increase energy efficiency, and minimize the environmental impact of SC operations. Hybrid models that employ ML can forecast energy consumption based on historical data and real-time inputs; this helps proactively plan energy needs and optimize energy use. [Sishi and Telukdarie \(2021\)](#) and [Vondra et al. \(2019\)](#) employed Monte Carlo simulation to train ML models for predicting energy consumption in SCs.

**Sustainability: Carbon emission auction** is a market-based approach to environmental sustainability, where SC entities engage in emissions trading to meet regulatory requirements and minimize their carbon footprint. This approach provides financial incentives for companies to reduce emissions and transition to more sustainable practices, making it an essential tool for addressing climate change within the SC ([Sandor et al., 2002](#)). Sim-ML models first use simulation to capture the dynamics of a carbon auction market and then apply ML to assist in setting the bidding price and volume. [Esmaeili Avval et al. \(2022\)](#) employed RL to set bidding prices and volume in a carbon auction market, which was modeled using the ABS technique.

**Sustainability: Investment** decisions refer to the financial resources allocated to various aspects of the SC operations. These investments can include capital expenditures in infrastructure, technology, and equipment to enhance SC efficiency. SC investments are made to improve processes, reduce costs, and enhance flexibility;

**Table 12**  
Subclasses of the sustainability driver.

Subclass	Description	Publications
Energy consumption planning	Managing the use of energy throughout the SC.	<a href="#">Sishi and Telukdarie (2021)</a> , <a href="#">Vondra et al. (2019)</a> , <a href="#">Behnamfar et al. (2022)</a>
Carbon emission auction	Understanding auction dynamics.	<a href="#">Esmaeili Avval et al. (2022)</a>
Investment	Predicting SC investment.	<a href="#">Bush et al. (2017)</a>
Circular economy	Analyzing different circular economy scenarios.	<a href="#">Walzberg et al. (2022)</a>

ultimately, such investments help achieve better SC performance. Sim-ML models can reduce the computational time needed to predict SC investment decisions by leveraging the advantages of Sim and ML. [Bush et al. \(2017\)](#) trained a deep learning model using the data generated by SD simulation to investigate the reaction of the investment community to the deployment of bioenergy given current technological development. They showed that the deep learning model was faster than the Sim in predicting the SC investment decisions.

**Sustainability: Circular Economy** is an economic system designed to be regenerative and restorative, rather than the traditional linear “take, make, dispose” model. In a circular economy, resources are used efficiently, waste and emissions are minimized, and products and materials are used for as long as possible. A Sim-ML model can capture the dynamic and intricate nature of circular economy systems using simulation while leveraging the predictive capabilities of ML ([Charnley et al., 2019](#)). This synergy allows for a more comprehensive analysis of various scenarios, considering resource flows, waste management, and the impact of different policies or technological interventions. [Walzberg et al. \(2022\)](#) integrated ABS and ML to identify the most effective circular economy strategies for reducing the landfill rate in wind blade (end-of-life blades of wind turbines) SCs.

#### 4.2. SIM-ML criterion: modeling techniques and algorithms

The modeling techniques and algorithms criterion refers to simulation and ML approaches. However, some studies have ventured further and also explored optimization techniques. The Sim-ML criterion for modeling techniques and algorithms consists of twelve Sim-ML Classes, six of which refer to the different combinations of hybrid Sim-ML methods, and the remaining six extend the original classification of hybrid models presented by [Mustafee et al. \(2020\)](#). As discussed in [Section 1.1](#), the original classification included only Model Type A-E, with Types A-C mapped to the three predominant formats of hybrid simulation, Type D and E as two forms of hybrid models. However, [Mustafee et al. \(2020\)](#) did not consider optimization in their methodological assessment of the modeling approaches; in this paper, we consider optimization.

**Table 13**  
Subclasses of DiscreteSimulation-ML and DiscreteSimulation-ML-Optimization.

	Subclass	Description	Publications
Discrete Methodology	DES-SL	Training supervised learning (SL) models using data generated by discrete event simulation (DES).	<a href="#">Badakhshan and Ball (2023)</a> , <a href="#">Priore et al. (2019)</a> , <a href="#">Carbonneau et al. (2008)</a> , <a href="#">Mukherjee et al. (2022)</a> , <a href="#">Badakhshan et al. (2022)</a> , <a href="#">Greis et al. (2022)</a> , <a href="#">Ktenioudaki et al. (2021)</a> , <a href="#">Shayeez et al. (2021)</a> , <a href="#">Jackson et al. (2021)</a> , <a href="#">Emerson and Piramuthu (2004)</a>
	DES-UL	Employing DES to assess the impact of disruptions identified by unsupervised learning (UL) models on SC performance.	<a href="#">Weihrach et al. (2018)</a>
	DES-RL	Training reinforcement learning (RL) models using data generated by DES.	<a href="#">Serrano-Ruiz et al. (2022)</a> , <a href="#">Afridi et al. (2020)</a> , <a href="#">Pan (2008)</a> , <a href="#">Rao et al. (2003)</a> , <a href="#">Lang et al. (2020)</a> , <a href="#">Creighton and Nahavandi (2002)</a> , <a href="#">Idrees et al. (2006)</a> , <a href="#">Zhang et al. (2018)</a> , <a href="#">Waschneck et al. (2018)</a> , <a href="#">El Shar et al. (2022)</a> , <a href="#">Xiang (2020)</a> , <a href="#">Yang et al. (2015)</a> , <a href="#">Xu et al. (2009)</a> , <a href="#">Dahlem and Harrison (2010)</a> , <a href="#">Sheremetov and Rocha-Mier (2008)</a> , <a href="#">Kim et al. (2005)</a>
	ABS-SL	Training SL models using data generated by agent-based simulation (ABS). Using SL to predict input parameters for ABS models.	<a href="#">Walzberg et al. (2022)</a> , <a href="#">Etemadidavan and Collins (2022)</a> , <a href="#">Gruzauskas et al. (2019)</a> , <a href="#">Kiekintveld et al. (2007)</a> , <a href="#">Pardoe and Stone (2007)</a> , <a href="#">Pardoe and Stone (2004)</a> , <a href="#">Pardoe and Stone (2004)</a>
	ABS-RL	Training RL models using data generated by ABS.	<a href="#">Wang et al. (2022)</a> , <a href="#">Zou et al. (2022)</a> , <a href="#">Du and Xiao (2019)</a> , <a href="#">Lee and Sikora (2019)</a> , <a href="#">Jinqi et al. (2017)</a> , <a href="#">Mortazavi et al. (2015)</a> , <a href="#">Saitoh and Utani (2013)</a> , <a href="#">Kim et al. (2010)</a> , <a href="#">Jiang and Sheng (2009)</a> , <a href="#">Kwon et al. (2008)</a> , <a href="#">Zhang and Bhattacharyya (2007)</a> , <a href="#">Li et al. (2006)</a> , <a href="#">Sheremetov et al. (2005)</a> , <a href="#">Ravulapati et al. (2004)</a> , <a href="#">Okada et al. (2023)</a> , <a href="#">Yang et al. (2022)</a> , <a href="#">Esmaili Avval et al. (2022)</a> , <a href="#">Kosasih and Brintrup (2022)</a> , <a href="#">Hirano et al. (2021)</a> , <a href="#">Barat et al. (2019a)</a> , <a href="#">Yang et al. (2022)</a> , <a href="#">Aghaie and Hajian Heidary (2019)</a> , <a href="#">Barat et al. (2019b)</a> , <a href="#">Kaihara and Fujii (2008)</a> , <a href="#">Lin and Pai (2000)</a>
Optimization	DES-SL-OPT	Determining optimal SC decisions by integrating optimization (OPT) with DES and SL.	<a href="#">Guo et al. (2023)</a> , <a href="#">Raghuram et al. (2022)</a> , <a href="#">Ben Kacem et al. (2020)</a> , <a href="#">Badakhshan and Ball (2024)</a>
	ABS-RL-OPT	Determining optimal SC decisions by integrating optimization (OPT) with ABS and RL.	<a href="#">Gutierrez-Franco et al. (2021)</a> , <a href="#">Liu et al. (2011)</a>

In the remainder of this section, the two categories of Sim-ML Classes (i.e., with and without optimization) are discussed under the same section for better readability. The acronyms used in this section are DES for discrete-event simulation, ABS – agent-based simulation, SD – system dynamics, MCS – Monte Carlo simulation, SL – supervised learning, UL – unsupervised learning, RL – reinforcement learning, OPT for optimization.

##### 4.2.1. Sim-ML class: discrete simulation methods with ML & Sim-ML class: discrete simulation methods with ML and optimization

Combining discrete simulation techniques like DES and ABS with ML methods and optimization approaches in a single modeling framework creates a powerful tool for solving complex SCM problems. They provide a more holistic and adaptable solution to real-world SC problems characterized by dynamic and uncertain conditions. [Table 13](#) lists the subclasses of two Sim-ML Classes: Discrete simulation-ML Class and Discrete simulation-ML-optimization Class.

The Discrete Simulation-ML Class includes five subclasses: DES-SL, DES-UL, DES-RL, ABS-SL and ABS-RL. These are discussed next.

**DiscreteSimulation-ML: DES-SL** subclass is assigned to studies integrating DES and SL. One key advantage of this integration is that DES can provide the data necessary to train SL models. For example, [Priore et al. \(2019\)](#) and [Carbonneau et al. \(2008\)](#) utilized data generated by DES to train SL models with the specific goal of minimizing the Bullwhip effect within the SC. Furthermore, [Mukherjee et al. \(2022\)](#) harnessed data from the DES to train an SL model, which, in turn, identified strategies for enhancing SC resilience when faced with disruptions. This integrated approach demonstrates the potential to leverage simulation data for improving SC performance and responsiveness.

**DiscreteSimulation-ML: DES-UL** subclass pertains to studies that combine DES with UL, often involving clustering techniques. A notable example of the subclass is the work by [Weihrach et al. \(2018\)](#), where the authors present a conceptual model in which UL is employed to identify disruptions through clustering analysis, with DES used to assess disruptions’ effects on SC performance. This integrated approach allows for a more in-depth exploration of disruptions’ impacts within the SC.

**DiscreteSimulation-ML: DES-RL** entails the utilization of DES to facilitate the training of RL models. Notable instances of this approach include the work of [El Shar et al. \(2022\)](#) and [Yang et al. \(2015\)](#), where DES played a pivotal role in training RL models to tackle intricate challenges in inventory planning. Further studies related to the subclass include the work by [Yanchun \(2008\)](#), who harnessed DES to train an RL model, enabling the determination of optimal order quantities and distribution strategies within the SC.

**DiscreteSimulation-ML: ABS-SL** encompasses two main approaches: training SL models using data generated by ABS models and using supervised learning to estimate input parameters for ABS models. For instance, [Kiekintveld et al. \(2007\)](#) and [Pardoe and Stone \(2007\)](#) employed ABS-generated data to train SL algorithms for price prediction. In another application, [Gruzauskas et al. \(2019\)](#) employed an ANN to forecast demand and subsequently incorporated these predictions into an ABS model to predict food waste.

**DiscreteSimulation-ML: ABS-RL** refers to studies that use ABS to train an RL agent. [Kosasih and Brintrup \(2022\)](#) and [Wang et al. \(2022\)](#) developed an ABS environment in which the RL agent learns optimal inventory replenishment strategies. [Lee and Sikora \(2019\)](#) trained an RL agent for supplier selection and production planning using ABS-generated data.

The Discrete Simulation-ML-Optimization Class includes two subclasses: DES-SL-OPT and ABS-RL-OPT.

**DiscreteSimulation-ML-Optimization: DES-SL-OPT** subclass identifies studies that enhance the effectiveness of DES-SL models by incorporating optimization techniques. For instance, in the study by [Ben Kacem et al. \(2020\)](#), a Genetic Algorithm (GA) was applied to their DES-SL model to optimize resource allocation within a healthcare SC. Additionally, [Badakhshan and Ball \(2024\)](#), used a mixed-integer programming model integrated with a DES-SL framework to determine the optimal master production schedule for an SC.

**DiscreteSimulation-ML-Optimization: ABS-RL-OPT** refers to studies that integrated optimization with ABS-RL models. This integration results in identifying optimal SC decisions. [Gutierrez-Franco et al. \(2021\)](#) used optimization to identify the best resource allocation and then created an ABS environment for an RL agent to learn the optimal routes in a vehicle route planning problem. [Liu et al. \(2011\)](#) integrated a GA with ABS-RL to identify the optimal price for a retailer in a two-echelon SC.

#### 4.2.2. Sim-ML class: continuous simulation methods with ML & Sim-ML class: continuous simulation methods with ML and optimization

The Continuous Simulation-ML Class and the Continuous Simulation-ML-Optimization Class each include only one subclass, namely, SD-SL and SD-SL-OPT. These are discussed next ([Table 14](#)).

**ContinuousSimulation-ML: SD-SL** subclass is assigned to studies that use SD simulation to train an SL model. [Roorkhosh et al. \(2023\)](#) trained an artificial neural network (ANN) using the data generated by the SD simulation to improve SC resilience. [Jaenichen et al. \(2022\)](#) and [Kurian et al. \(2023\)](#) employed tree-based algorithms, trained using SD simulation-generated data, to reduce the Bullwhip effect.

**ContinuousSimulation-ML-Optimization: SD-SL-OPT** subclass identifies studies incorporating optimization techniques that enhance the effectiveness of SD-SL models. [Chi et al. \(2007\)](#) and [Corsini et al. \(2022\)](#) provide the implementation of enhanced SD-SL models for optimizing replenishment policies within SCs by employing Particle

Swarm and GA, respectively.

#### 4.2.3. Sim-ML class: Monte Carlo methods with ML & Sim-ML class: Monte Carlo methods with ML and optimization

The Monte Carlo Methods-ML Class includes the subclasses MCS-SL and MCS-RL. Its optimization counterpart of this Class, namely, the Monte Carlo Methods-ML-Optimization Class, only includes the MCS-UL-OPT subclass. These are discussed next ([Table 15](#)).

**MonteCarlo-ML: MCS-SL** subclass is assigned to studies that use MCS to train SL. MCS models the probability of different outcomes through repeated random sampling. In the case of SC modeling, MCS sample from probability distributions that represent SC uncertainties, thereby providing a diverse range of training data for ML models. [Sishi and Telukdarie \(2021\)](#) and [Vondra et al. \(2019\)](#) applied MCS-SL for energy consumption planning in the SC.

**MonteCarlo-ML: MCS-RL** refers to studies that use MCS to train RL models. [Rana and Oliveira \(2014\)](#) used MCS to train an RL agent in the optimal pricing strategies in a dynamic SC environment. [Mehta and Yamparala \(2014\)](#) used the data generated by MCS to train an RL agent for determining order quantities.

**MonteCarlo-ML-Optimization: MCS-UL-OPT** corresponds to studies using MCS and UL to enhance computational efficiency in solving optimization problems. [Jacobson et al. \(2021\)](#) and [Karimi-Mamaghan et al. \(2020\)](#) integrated MCS and K-means clustering with the sample average approximation (SAA) and iterated local search (ILS) algorithms, respectively, to enhance the computational efficiency in identifying the optimal SC decisions.

#### 4.2.4. Sim-ML class: hybrid simulation with ML & Sim-ML class: hybrid simulation with ML and optimization

Our literature review identified studies that employed two or more simulation techniques, i.e., hybrid simulation ([Brailsford et al., 2019](#)), to capture the dynamics of the SC. Each simulation technique can represent various aspects of the SC, ranging from micro-level details to macro-level behaviors. Integrating these techniques leads to a more realistic representation of the SC dynamics. The Hybrid Simulation-ML Class includes six subclasses ([Table 16](#)). For example, [Cavalcante et al. \(2019\)](#) used the K-nearest neighbor algorithm trained on data generated by DES, SD, and ABS to classify suppliers (HybridSimulation-ML: DES-SD-ABS-SL); [Wang et al. \(2020\)](#) combined DES and SD to generate data for principal component analysis (HybridSimulation-ML: DES-SD-UL); [Clark and Kulkarni \(2021\)](#) integrated DES, ABS, and SD to train an RL agent for inventory planning (HybridSimulation-ML: DES-SD-ABS-RL).

The HybridSimulation-ML-Optimization Class includes only two subclasses ([Table 16](#)) for the two studies that used hybrid simulation with ML and OPT. [Behnamfar et al. \(2022\)](#) integrated DES and SD with particle swarm optimization to generate data for an ANN that predicted the permissible emission limit (HybridSimulation-ML-Optimization: DES-SD-SL-OPT). [Pereira and Frazzon \(2021\)](#) used an ANN for demand forecasting and then incorporated a Genetic Algorithm into a DES-ABS model to identify the optimal replenishment policies in an omnichannel retail SC (HybridSimulation-ML-Optimization: DES-ABS-SL-OPT).

#### 4.2.5. Sim-ML class: simulation model with ML & Sim-ML class: simulation model with ML and optimization

The hybrid Simulation Model (SM) and ML class (SM-ML) include two subclasses; its counterpart (SM-ML-OPT) has three subclasses

**Table 14**  
Subclasses of ContinuousSimulation-ML and ContinuousSimulation-ML-Optimization.

	Subclass	Description	Publications
Continuous Methodology	SD-SL	Training supervised learning (SL) models using data generated by system dynamics (SD) simulation.	<a href="#">Roorkhosh et al. (2023)</a> , <a href="#">Bush et al. (2017)</a> , <a href="#">Jaenichen et al. (2022)</a> , <a href="#">Kurian et al. (2023)</a>
	Optimization	SD-SL-OPT Determining optimal SC decisions by integrating optimization (OPT) with SD and SL	<a href="#">Chi et al. (2007)</a> , <a href="#">Corsini et al. (2022)</a>

**Table 15**  
Subclasses of MonteCarlo-ML and MonteCarlo-ML-Optimization.

	Subclass	Description	Publications
Monte Carlo Methods	MCS-SL	Training SL models using data generated by Monte Carlo simulation (MCS).	Sishi and Telukdarie (2021), Vondra et al. (2019)
	MCS-RL	Training RL models using data generated by MCS.	Rana and Oliveira (2014), Mehta and Yamparala (2014), Tuncel et al. (2014), Cao (2003)
	Optimization	MCS-UL- OPT	Enhancing computational efficiency in solving optimization problems by integrating optimization with MCS and UL.

**Table 16**  
Subclasses of HybridSimulation-ML and HybridSimulation-ML-Optimization.

	Subclass	Description	Publications
Hybrid Simulation	DES-SD-SL	Training SL models using data generated by DES and SD.	Sankaran et al. (2022)
	DES-SD-UL	Training UL models using data generated by DES and SD.	Wang et al. (2020)
	DES-MCS-RL	Training RL models using data generated by DES and MCS.	Gros et al. (2020)
	SD-ABS-RL	Training RL models using data generated by SD and ABS.	Zhou et al. (2015)
	ABS-MCS-SL	Training SL models using data generated by ABS and MCS.	Bodendorf et al. (2022)
	DES-SD-ABS-RL	Training RL models using data generated by DES, SD, and ABS.	Clark and Kulkarni (2021)
	DES-SD-ABS-SL	K-Nearest Neighbors (K-NN) is first used to cluster data generated by DES, SD, and ABS models before being used in logistic regression. K-NN and logistic regression are both SL.	Cavalcante et al. (2019)
	Optimization	DES-SD-SL- OPT	Training SL models with data generated by DES, SD, and OPT.
	DES-ABS- SL-OPT	Using SL to predict input parameters to DES-ABS models and then employing OPT to identify optimal SC decisions.	Pereira and Frazzon (2021)

**Table 17**  
Subclasses of Simulation Model (SM)\*-ML and SM-ML-Optimization.

	Subclass	Description	Publications	
Other Simulation Approaches	SM-SL	Training SL models using data generated by simulation. Using SL to predict input parameters for simulation models.	Liebenberg and Jarke (2023), Schnieder et al. (2023)	
	SM-RL	Training RL models using data generated by simulation.	Sui et al. (2010), Li et al. (2008)	
	Optimization	SM-SL- OPT	Using OPT to enhance solution space exploration of SL models that are trained by simulation-generated data.	Lei et al. (2000a), Lei et al. (2000b)
		SM-UL- OPT	Enhancing computational efficiency in solving optimization problems by integrating optimization with simulation and UL.	Zdolsek Draksler et al. (2023)
		SM-RL- OPT	Using OPT to enhance solution space exploration of RL models that are trained by simulation-generated data.	Serrano-Ruiz et al. (2021), Zhou and Zhou (2019)

Note (Table 17): \* The term simulation model (SM) is used in this subclass without specifying the applied simulation technique, as the authors have not explicitly mentioned the technique.

(Table 17). The term simulation model (SM) is employed in this subclass without specifying the applied simulation technique, as the authors have not explicitly mentioned a technique. However, there is an exception noted in the study by Liebenberg and Jarke (2023), where Finite Element Method (FEM) was applied to simulate manufacturing processes.

**Simulation-ML: SM-SL** subclass is assigned to studies that utilize simulation techniques other than DES, SD, ABS, and MCS, as well as studies that do not specify the simulation technique. These studies either employ simulation for training or testing SL models or predict simulation parameters using SL and incorporate them into the simulation model. For example, Liebenberg and Jarke (2023) utilized the Finite Element Method (FEM) to train an artificial neural network (ANN) for production scheduling.

**Simulation-ML: SM-RL** subclass encompasses studies that utilize simulation techniques other than DES, SD, ABS, and MCS, as well as studies that do not specify the simulation technique used. These studies either employ simulation for training or testing RL models or predict simulation parameters using SL and incorporate them into the simulation model. Sui et al. (2010) and Guo et al. (2023) trained an RL agent for inventory planning using data generated through simulation. Schnieder et al. (2023) applied SL for demand prediction and integrated the forecasted demand into a simulation model.

**Simulation-Optimization-ML: SM-SL-OPT** studies pertain to research that incorporates simulation and optimization into the frameworks of SL but does not specify the employed simulation technique. Lei et al. (2000a) and Lei et al. (2000b) integrated evolutionary algorithms with rule learning techniques to guide identifying decision rules (SL) for selecting SC partners.

**Simulation-Optimization-ML: SM-UL-OPT** refers to studies that use simulation and UL to enhance computational efficiency in solving optimization problems. Zdolsek Draksler et al. (2023) integrated the minimal k-cut clustering algorithm and simulation with the Tabu search heuristics to enhance the computational efficiency in addressing a vehicle routing problem.

**Simulation-Optimization-ML: SM-RL-OPT** studies pertain to research that incorporates simulation and optimization into the frameworks of RL but does not specify the employed simulation technique. Zhou and Zhou (2019) incorporated a scatter search algorithm into an RL model, trained on simulated data to guide solution space exploration.

#### 4.2.6. Sim-ML class: hybrid ML with discrete simulation methods

Our review identified two studies that used a hybrid ML approach (i. e., SL + RL and SL + UL) and used it together with discrete simulation methods. SL is an efficient tool for predicting external parameters, such as customer demand, which helps an RL agent make informed decisions.



Zhang et al. (2013) used demand forecast by an SL algorithm as an input to a DES model, which was used to train an RL agent for inventory planning. Starting with UL followed by SL aids in data preprocessing, leading to more accurate SL models. Pereira et al. (2018) first clustered demand data to improve demand forecast accuracy and then used an ANN to predict the demand. The two subclasses of HybridML-DiscreteSimulation are listed in Table 18.

#### 4.3. SIM-ML criterion: data flow mechanisms

Section 4.2 categorizes hybrid models that combine various simulation, optimization, and ML techniques into Sim-ML subclasses. However, it is also essential to consider the data flow (DF) mechanisms for data exchange between the sub-components of a hybrid model. Understanding these mechanisms is crucial because the effectiveness of a hybrid model depends not only on the integration of different methodologies but also on how data is shared and processed among them. Our literature review identified four distinct Sim-ML classes related to data flow: sequential, feedback, sequential-feedback, and feedback-sequential.

##### 4.3.1. SIM-ML class: sequential data flow

Sequential data flow refers to a step-by-step approach where different components of a hybrid model are applied one after another in a predefined sequence. Each modeling technique may address a specific aspect or part of the problem, and the outputs of one technique may serve as inputs to the next. The goal is to improve overall performance and accuracy (Mooney & Roddick, 2013). The SIM-ML subclasses are described next, with the literature synthesis presented in Table 19. The various forms of data flows are mapped to specific data flow (DF) types.

**Sequential Data Flow: ML followed by simulation (DF Type A)** consists of studies that use ML techniques to forecast uncertain parameters, such as demand, based on historical data and other relevant information. Once these forecasts are generated, they are incorporated as inputs into a simulation model, allowing for a more accurate and data-driven simulation of the system's behavior. Pereira et al. (2018) and Gruzauskas et al. (2019) addressed the inventory planning problem by predicting demand using ANN and using this as input to simulation models. Weihrauch et al. (2018) developed a conceptual model that used ML to identify disruptions and conduct scenario analysis using simulation.

**Sequential Data Flow: Simulation followed by ML (DF Type B)** subclass identifies studies that use the data generated by simulation to train an ML model. This approach can benefit an ML algorithm by helping it learn complex patterns, relationships, and trends that may not be immediately apparent. The Type B approach is widely used in the literature. For instance, Sankaran et al. (2022) used the data generated by DES to train a recurrent neural network to predict product return. Ktenioudaki et al. (2021) employed a boosted regression tree, trained on DES-generated data, to predict waste in a perishable food SC. Jackson et al. (2021) used the data generated by DES to train an ANN to classify inventory replenishment policies.

**Sequential Data Flow: ML followed by simulation-based optimization (DF Type C)** refers to studies that employ ML techniques to forecast uncertain parameters and subsequently incorporate these predictions into a simulation-based optimization (SBO) model, with the

**Table 18**  
Subclasses (SL-DES-RL and DES-ABS-UL-SL) of the Sim-ML Class HybridML-DiscreteSimulation.

Subclass	Description	Publications
SL-DES-RL	Using SL to predict input parameters to DES and then training RL models by DES.	Zhang et al. (2013)
DES-ABS-UL-SL	Using UL to cluster data generated by DES and ABS, followed by prediction by SL.	Pereira et al. (2018)

latter determining the optimal values of the decision parameters. By combining SBO, which can efficiently explore potential solutions and identify the optimal solution, with the predictive capabilities of ML, this methodology enhances the accuracy and efficiency of decision-making processes in SCs, leading to improved performance and efficient resource allocation. Raghuram et al. (2022) and Pereira and Frazzon (2021) inputted the forecasted demands by ML into SBO models that determined the optimal inventory decisions.

**Sequential Data Flow: Simulation-based optimization followed by ML (DF Type D)** regards studies that generate Pareto optimal solutions for ML models. Behnamfar et al. (2022) trained an ANN to predict the permissible emission limit using the Pareto set generated by SBO.

**Sequential Data Flow: Simulation followed by ML followed by optimization (DF Type E)** represents the following two categories of studies.

ML models are trained using simulation-generated data. These models are then optimized by identifying their optimal input parameters using algorithms like Particle Swarm Optimization (Corsini et al., 2022) or Genetic Algorithms (Chi et al., 2007). This process enhances computational efficiency in determining optimal SC decisions.

ML is employed to update optimization model constraints in response to disruptions. This approach helps minimize the impact of disruptions on SC performance. For example, Badakhshan and Ball (2024) used ML to adjust minimum inventory levels at SC members in response to demand and lead time disruptions.

**Sequential Data Flow: ML followed by simulation followed by optimization (DF Type F)** subclass aligns with data flow mechanisms that begin with ML for predicting input parameters within a simulation model, followed by using simulation outputs as input parameters in an optimization model to determine optimal SC decisions. This method harmonizes data-driven insights from ML, realistic simulations, and optimization, ultimately improving SC service levels and profitability. Guo et al. (2023) successfully employed this approach to tackle an inventory and scheduling problem related to a reusable transport item, demonstrating its ability to enhance service levels and profitability.

##### 4.3.2. Sim-ML class: feedback data flow

Feedback data flow enables information to flow from one model component to another in a loop. This mechanism allows the hybrid model to adjust its behavior based on the results obtained from the sub-components of the model. Table 20 shows subclasses for feedback data flow.

**Feedback Data Flow: Reinforcement learning (RL) coupled with simulation (DF Type G)** refers to studies that use RL with simulation. They employ simulation to create an environment where the reinforcement learning agent can interact and learn from its experiences. Simulation provides a realistic representation of the SC dynamics that improves the quality of data for RL. RL agents can experiment and learn within the simulated environment without real-world consequences. This is particularly valuable in SCM, where poor decisions can lead to costly disruptions. Different simulation techniques have been used to train reinforcement learning models: ABS (e.g., Wang et al., 2022; Zou et al., 2022), DES (e.g., Afridi et al., 2020; Carbonneau et al., 2008; Lang et al., 2020), MCS (e.g., Rana & Oliveira, 2014; Tuncel et al., 2014). However, our literature review has not identified any existing work that has employed SD for training RL models. This can be attributed to several reasons. Firstly, developing accurate SD models requires expertise and domain knowledge as these models tend to be complex, with many interconnected variables and equations representing SC dynamics. Secondly, ensuring that the SD model accurately represents the intricacies of a specific SC can be difficult. Mismatches between the model and real-world SC behavior can result in suboptimal RL policies. Thirdly, defining a meaningful and computationally efficient reward function for RL in complex SD simulation models can be challenging.


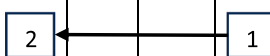
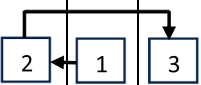
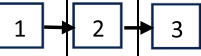
**Feedback Data Flow: Reinforcement learning (RL) coupled with simulation and heuristics (DF Type H)** corresponds to studies that

**Table 19**  
Subclasses of the Sim-ML Class called Sequential Data Flow.

Subclass	ML	SIM	OPT	SBO	Description	Publications
ML followed by simulation <b>(DF Type A)</b>	1 →	2			Forecasting uncertain parameters through ML and subsequently conducting scenario analysis using simulation.  Detecting disruptions through ML and subsequently conducting scenario analysis using simulation.	Weihrauch et al. (2018), Pereira et al. (2018), Gružauskas et al. (2019)
Simulation followed by ML <b>(DF Type B)</b>	← 2	1			Training ML models using data generated by simulation.	Emerson and Piramuthu (2004), Liebenberg and Jarke (2023), Roozkhosh et al. (2023), Badakhshan and Ball (2023), Badakhshan et al. (2022), Serrano-Ruiz et al. (2022), Bodendorf et al. (2022), Zou et al. (2022), Priore et al. (2019), Bush et al. (2017), Carbonneau et al. (2008), Sankaran et al. (2022), Etemadidavan and Collins (2022), Ktenioudaki et al. (2021), Shayeez and Panicker (2021), Sishi and Telukdarie (2021), Jackson and Velazquez-Martinez (2021), Wang et al. (2020), Cavalcante et al. (2019), Vondra et al. (2019), Kiekintveld et al. (2007), Pardoe and Stone (2007), Pardoe and Stone (2004), Schnieder et al. (2023), Kurian et al. (2023), Okada et al. (2023), Greis et al. (2022), Mukherjee et al. (2022), Jaenichen et al. (2022), Pardoe and Stone (2005)

(continued on next page)

Table 19 (continued)

ML followed by simulation-based optimization (SBO) <b>(DF Type C)</b>			Forecasting uncertain parameters through ML and subsequently identifying optimal SC decisions using SBO.	Raghuram et al. (2022), Pereira and Frazzon (2021)
SBO followed by ML <b>(DF Type D)</b>			Training ML models using data generated by SBO.	Behnamfar et al. (2022)
Simulation followed by ML followed by optimization <b>(DF Type E)</b>			Training ML models using data generated by simulation and subsequently optimizing the input parameters to ML models.  Using ML to update optimization constraints in line with disruptions.	Chi et al. (2007), Corsini et al. (2022), Ben Kacem et al. (2020), Lei et al. (2000a), Lei et al. (2000b), Jacobson et al. (2021), Karimi-Mamaghan et al. (2020), Zdolsek Draksler et al. (2023), Badakhshan and Ball (2024)
ML followed by simulation followed by optimization <b>(DF Type F)</b>			Forecasting uncertain parameters through ML, subsequently conducting scenario analysis using simulation, and then identifying optimal SC decisions using optimization.	Guo et al. (2023)

combine a metaheuristic with RL. Metaheuristics are crucial in balancing the exploration–exploitation trade-off, helping the RL agent make informed decisions. This reduces the number of exploratory trials required for the agent to learn optimal policies. For example, Serrano-Ruiz et al. (2021) proposed a conceptual framework integrating RL and heuristics to address a master production scheduling problem. In another instance, Liu et al. (2011) coupled a GA with ABS-RL to

determine the optimal price for a retailer in a two-echelon SC. Zhou and Zhou (2019) integrated the scatter search algorithm with an RL model trained on simulated data to optimize inventory decisions.

4.3.3. Sim-ML class: sequential-feedback data flow

The Sim-ML class on sequential-feedback refers to integrating sequential and feedback data flows. This involves a two-step approach

where sequential and feedback data flows are applied one after another in a predefined sequence. Table 21 shows subclasses for sequential-feedback data flow.

**Sequential-feedback Data Flow: RL followed by optimization (DF Type I)** entails training of RL models using simulation data, followed by the utilization of optimization techniques to determine the optimal SC decisions. These decisions consider constraints learned by the RL model during the training process. For instance, Esmaeili Avval et al. (2022) applied this approach by initially using RL to determine the bidding price and volume for an SC in the carbon auction market. Subsequently, they incorporated these RL-learned constraints into an optimization model, facilitating the identification of optimal tactical and operational decisions.

**Sequential-feedback Data Flow: Optimization followed by training RL model using simulation data (DF Type J)** involves using simulation or optimization as a preprocessing step before training an RL model. This approach can significantly reduce the computational burden on the RL model, making the analysis more time-efficient. For instance, Gutierrez-Franco et al. (2021) employed optimization to initially determine the optimal allocation of resources and then created an ABS environment for an RL agent to learn the optimal routes in a vehicle route planning problem. In many RL models, the agent lacks complete information about the state of the environment. Bayesian networks can be used to estimate the current state based on available observations, providing the RL agent with more informed decisions. Zhou et al. (2015) utilized a Bayesian network to estimate the likelihood of various states based on simulation data. These estimates were then incorporated into the RL agent's training process.

#### 4.4. Sim-ML criterion: industry 4.0 technologies

Industry 4.0 technologies are the enablers of the Fourth Industrial Revolution. These technologies refer to advanced digital and automated technologies that are transforming various industries and revolutionizing how businesses operate. Industry 4.0 technologies are characterized by their ability to collect, analyze, and utilize large amounts of data to improve efficiency, productivity, and decision-making (Duan et al., 2021). Ruel et al. (2023) used a decision-oriented approach to categorize Industry 4.0 technologies into two groups. The first category comprises operational technologies, which include sensors, actuators, robotics, self-driving vehicles, and the Internet of Things (IoT). The second category comprises support technologies like data analytics and blockchain. The classification framework by Ruel et al. (2023) provides a valuable foundation by categorizing support technologies in SCM. However, their framework does not fully encompass the rapidly evolving landscape of digital technologies integral to modern supply chains. Specifically, it overlooks digital twins, which are increasingly essential for creating digitally integrated supply chain environments. However, our classification framework includes digital models, digital shadows, and digital twins, deepening our understanding of how hybrid models can drive digitally integrated supply chain environments.

##### 4.4.1. Sim-ML class: support technologies

Support technologies offer valuable capabilities for SCs, encompassing improved decision-making, enhanced efficiency, risk reduction, and novel opportunities for automation and optimization. Their adoption can enhance the competitiveness and resilience of SCs. Table 22 provides an overview of the subclasses of support technologies and their respective publications.

**Support Technologies: Digital Model.** A digital model is a computerized representation of elements, processes, and components within the SC ecosystem. It uses historical data to create a virtual replica of the real-world SC. The primary goal of digital SC models is to capture the intricacies of the SC, empowering businesses to analyze operations and make well-informed decisions. However, digital models lack real-time or near real-time monitoring capabilities, making them less

responsive to environmental changes and unable to update SC decisions promptly. Kim et al. (2010) and Kosasih and Brintrup (2022) presented digital models for inventory planning problem. Rana and Oliveira (2014) and Du and Xiao (2019) developed digital models to identify the optimal pricing policies.

**Support Technologies: Digital Shadow.** A digital shadow is a virtual representation of a physical object, system, or process created in real time using data collected from sensors, IoT devices, and other sources (Kritzinger et al., 2018). Digital shadows are continuously updated to reflect changes in the physical entity they represent. They serve primarily for data collection and predictive analysis, with a one-way interaction, i.e., gathering data from the physical entity without directly controlling its action. Wang et al. (2020) developed a digital shadow to detect SC disruptions.

**Support Technologies: Digital Twin.** A digital twin is a virtual representation of a physical object, process, or system that mimics the real-world counterpart using data from sensors, IoT devices, and other sources. The digital twin interacts bidirectionally with its physical counterpart, allowing for real-time monitoring, analysis, simulation, optimization, and control (Badakhshan & Ball, 2021). Digital twins are used in SCs to improve efficiency and enhance overall performance (Ball & Badakhshan, 2022). Weihrauch et al. (2018) proposed a digital twin for SC process control in which disruptions are identified, and SC decisions are updated to minimize the impact of the disruptions on SC performance. Waschneck et al. (2018) presented a digital twin that updated production schedules according to real-time data collected from the production floor. Badakhshan and Ball (2023) used a digital twin to identify policies that reduced the SC cash conversion cycle.

**Support Technologies: Blockchain.** Blockchain is a decentralized and distributed digital ledger technology that securely records transactions across multiple computers or nodes. Blockchain can enhance transparency, traceability, and efficiency in various stages of the SC. By leveraging blockchain, SC members can securely record and share data related to the movement of goods, information, and payments in a decentralized and tamper-resistant manner (Chang & Chen, 2020). This helps create a trusted and reliable system for managing SC processes and mitigating issues like fraud, counterfeiting, and lack of visibility (Dutta et al., 2020). Roozkhosh et al. (2023) used blockchain technology to improve SC resilience.

**Support Technologies: Cloud manufacturing.** Cloud manufacturing is a model that leverages cloud computing technologies to provide on-demand manufacturing services. In cloud manufacturing, various manufacturing resources, such as production equipment, software tools, and expertise, are made available as virtualized services over the Internet. This model allows manufacturers to access, use, and manage manufacturing resources remotely without requiring extensive in-house infrastructure. Cloud manufacturing offers scalability, cost efficiency, and collaboration, making it a flexible and efficient solution for modern manufacturing needs. Cloud manufacturing is particularly beneficial for small and medium-sized enterprises (SMEs) that may not have the resources to maintain extensive in-house manufacturing capabilities. It also promotes sustainability by optimizing resource utilization and reducing waste. Jinqi et al. (2017) addressed an inventory planning problem in an SC network in a cloud manufacturing environment.

#### 4.5. Sim-ML criterion: industrial sectors

This section categorizes articles identified in our dataset for the literature review based on the industrial sectors they target. While many publications focus on generic SCs involving suppliers, producers, retailers, and customers, some specifically address particular industries with unique SC requirements. Classifying publications to a single industry is not always straightforward, particularly for manufacturing and retail, as SCs often involve stakeholders from both areas. In such cases, we assign them to the industry that aligns with the publication's primary



**Table 20**  
Subclasses of feedback data flow.

Subclass	RL	SIM	HEU	Description	Publications
Reinforcement learning coupled with simulation <b>(DF Type G)</b>				Training reinforcement learning models using data generated by simulation.	Dahlem and Harrison (2010), Wang et al. (2022), Afridi et al. (2020), Du and Xiao (2019), Lee and Sikora (2019), Jinqi et al. (2017), Mortazavi et al. (2015), Rana and Oliveira (2014), Saitoh and Utani (2013), Sui et al. (2010), Kim et al. (2010), Kwon et al. (2008), Jiang and Sheng (2009), Li et al. (2008), Pan (2008), Zhang and Bhattacharyya (2007), Li and Zhao (2006), Sheremetov et al. (2005), Ravulapati et al. (2004), Rao et al. (2003), Lang et al. (2020), Creighton and Nahavandi (2002), Idrees et al. (2006), Zhang et al. (2018), Waschneck et al. (2018), Gros et al. (2020), Walzberg et al. (2022), Kosasih and Brintrup (2022), El Shar et al. (2022), Hirano et al. (2021), Clark and Kulkarni (2021), Barat et al. (2019a), Yang et al. (2019), Aghaie and Hajian Heidary (2019), Barat et al. (2019b), Yang and Zhang (2015), Mehta and Yamparala (2014), Tuncel et al. (2014), Zhang et al. (2013), Xu et al. (2009), Sheremetov and Rocha-Mier (2008), Kaihara and Fujii (2008), Kim et al. (2005), Cao (2003), Lin and Pai (2000), Xiang (2020), Yang et al. (2022)
Reinforcement learning coupled with simulation and heuristics <b>(DF Type H)</b>				Using metaheuristics to reduce the number of exploratory trials required for an RL agent.	Liu et al. (2011), Zhou and Zhou (2019), Serrano-Ruiz et al. (2021)

**Table 21**  
Subclasses of Sequential-Feedback Data Flow.

Subclass	RL	SIM	OPT	Description	Publications
Reinforcement learning followed by optimization <b>(DF Type I)</b>				Training an RL model using simulation data followed by optimization techniques to determine the optimal SC decisions.	Esmaeili Avval et al. (2022)
Optimization followed by training <b>(DF Type J)</b>				Identifying optimal resource allocation using optimization and subsequently training an RL agent in a simulated environment.	Zhou et al. (2015), Gutierrez-Franco et al. (2021)
an RL model using simulation data <b>(DF Type J)</b>				Estimating the current state using Bayesian networks and simulation data.	

focus. The *International Standard Industrial Classification* (ISIC), maintained by the United Nations (UNO, 2008), is the most used system for industrial sector classification. It divides industries into 21 sections, further categorized into divisions, groups, and classes. Table 23 presents the industry affiliations according to the ISIC sections; the sections are incorporated into our Sim-ML literature classification frameworks as Sim-ML classes and sub-classes. The five Sim-ML classes are described next based on UNO's (2008) definition:

**Manufacturing:** UNO (2008) defines manufacturing as comprising activities that involve converting materials, substances, or components into new products.

**Transportation and Storage:** Transportation and storage encompasses a wide range of activities related to transportation, logistics, and warehousing (UNO, 2008). The sector is characterized by its multifaceted nature, involving diverse modes of transport, complex supply chain networks, fluctuating demand, and a constant need for real-time decision-making.

**Electricity, gas, steam, and air conditioning:** The sector encompasses the generation, transmission, and distribution of electricity, as well as the production and distribution of gaseous fuels (natural gas, synthetic gas, and similar products), steam, and hot water for heating and other purposes. Additionally, it includes the provision of air conditioning and ventilation services (UNO, 2008).

**Wholesale and retail trade:** The sector refers to trade without transformation and covers a wide range of businesses, including wholesalers, retailers, and other intermediaries that facilitate the distribution of products to consumers. It is a fundamental sector in the economy as it deals with the final stages of the SC, ensuring that goods reach end consumers efficiently and conveniently.

**Human health and social work activities:** Include economic activities related to human healthcare and social services. This sector's distinctive features include the need for strict regulatory compliance, a wide range of product types, and varying demand patterns.

#### 4.5.1. Sim-ML class: manufacturing

In manufacturing, we identified the predominant use of hybrid models in electronics (with four studies on semiconductor SC) and in the food supply chain (seven studies). Table 21 shows Sim-ML subclasses for manufacturing. Semiconductor SC possesses distinctive characteristics

that shape its complexity and operational considerations. It is characterized by high globalization, long lead times, and short product life cycles. These make hybrid modeling a suitable approach for gaining insights, optimizing operations, and effectively addressing the challenges specific to this industry. Afridi et al. (2020) employed hybrid modeling to address the semiconductor SC's inventory planning and production scheduling problems. Weihrauch et al. (2018) and Jaenichen et al. (2022) applied hybrid modeling to improve the resilience of the semiconductor SC to disruptions.

Food SCs exhibit distinctive characteristics, including perishable and seasonal products, stringent regulatory requirements, diverse product ranges, and a need for effective quality control and traceability systems to ensure food safety. Hybrid modeling is particularly well-suited here due to the industry's dynamic and complex nature. Combining different modeling techniques, such as DES for production and distribution processes, with ML for demand forecasting and optimization for inventory management enables a comprehensive understanding of the SC. This approach helps address the unique challenges of the food industry by allowing for real-time monitoring and decision-making, enhancing efficiency, and supporting compliance with regulations. Zou et al. (2022) employed hybrid modeling to dynamically adjust delivery routes in the last mile of food delivery. Rana and Oliveira (2014) used hybrid modeling to identify optimal pricing strategies in a food SC. Barat et al. (2019a), Ktenioudaki et al. (2021), and Gruzauskas et al. (2019) applied hybrid modeling to minimize waste in food SCs.

#### 4.5.2. Sim-ML class: transportation and storage

Hybrid modeling allows for a comprehensive representation of the sector's intricate operations. It is particularly beneficial for tasks like route planning and warehouse operations, which are vital in ensuring the efficient movement and storage of goods and commodities. Zdolsek Drakler et al. (2023) and Schnieder et al. (2023) utilized hybrid modeling to address the last-mile delivery problem.

#### 4.5.3. Sim-ML class: electricity, gas, steam, and air conditioning

Hybrid modeling provides the flexibility to adapt to changing environmental conditions and optimize energy production and distribution processes, making it a suitable choice for modeling this sector while ensuring cost-effectiveness, sustainability, and uninterrupted energy

services. [Vondra et al. \(2019\)](#) used hybrid modeling to optimize production in biogas SCs.

#### 4.5.4. Sim-ML class: wholesale and retail trade

Hybrid modeling is an efficient choice for modeling this sector because it incorporates data-driven approaches for demand forecasting, customer behavior analysis, and inventory management while simultaneously employing optimization models to optimize logistics, pricing, and resource allocation. This versatility is crucial in a sector where responsiveness to changing market conditions, customer preferences, and SC efficiency is paramount. [Pereira and Frazzon \(2021\)](#) and [Pereira et al. \(2018\)](#) used hybrid modeling to synchronize demand and supply in omni-channel retail SCs. [Barat et al. \(2019b\)](#) used hybrid modeling to minimize waste and backlog for a food retailer.

#### 4.5.5. Sim-ML Class: human health and social work activities

Hybrid modeling can effectively address dynamic demand forecasting for various healthcare products while optimizing logistics and inventory management. This approach is vital for ensuring the availability of critical medical supplies, reducing costs, and maintaining the quality and safety of healthcare services. [Ben Kacem et al. \(2020\)](#) applied hybrid modeling to optimize resource allocation within a healthcare SC.

## 5. Discussion and conclusion

The synthesis of the literature using the Sim-ML literature classification framework has identified different objectives of employing hybrid models to address SC problems, the various forms of hybrid models, differences in dataflow among the constituent parts of the Sim-ML models, use of hybrid models with optimization methods, use of Industry 4.0 technologies to incorporate real-time elements to develop digital shadows and digital twins, and a plethora of opportunities in the application of the hybrid models to industrial use cases. In this section, we revisit the five top-level Sim-ML criteria defined in the framework ([Section 4](#)) and discuss some learnings and opportunities for future research.

### 5.1. SC drivers

To address RQ1, “*What are the main applications of hybrid modeling in SCM?*”, we analyzed the literature using the six supply chain drivers identified by [Chopra and Meindl \(2013\)](#) and introduced a seventh driver focused on sustainability. This addition allowed us to incorporate research on environmental and related themes into our analysis. The review revealed only six studies under the sustainability category, all of which were relatively recent studies. However, with the increasing focus on achieving Net-zero and Circular Economy goals, the application of hybrid modeling for sustainability is anticipated to grow significantly. Most studies were mapped to the inventory driver, with a balanced focus on customer-managed and vendor-managed inventory, as well as production planning and scheduling. This is consistent with the long-established use of simulation models in inventory management.

Our review identified only four papers focused on vehicle routing (transportation driver), all published between 2021 and 2023. The use of hybrid models in transportation offers decision-makers a comprehensive view of the network, enabling optimized routes, modes, and scheduling while considering cost, time, and other critical factors. Given the rise of the gig economy and the proliferation of ride-hailing, ride-sharing, and online delivery services such as Uber, LiftShare, and Deliveroo, hybrid models for vehicle routing are likely to gain increasing prominence.

In summary, while the application of hybrid models in traditional SCM areas like inventory management and production planning is well-established, there is significant potential for growth in underexplored areas such as sustainability and transportation. As these sectors evolve

and expand, hybrid modeling approaches will play an increasingly critical role in enhancing decision-making, optimizing operations, and supporting the broader goals of supply chain sustainability and efficiency.

### 5.2. SC modeling techniques and algorithms

To address RQ2, “*What are the most common hybrid modeling combinations used in SCM?*”, we analyzed the literature based on the underlying simulation methodology, viz, discrete, continuous, Monte Carlo methods (MCS), and the three forms of ML, namely SL, UL and RL. In addition, we considered whether optimization had been used in the hybrid study. A key finding was that several hybrid M&S-ML studies in our dataset also incorporated hybridity at the M&S or ML-technique level. The definition of *hybrid simulation*, *hybrid ML* and *hybrid model* is important in this context. Hybrid simulation is the mixing of simulation methods, e.g., DES + SD ([Brailsford et al., 2019](#)); hybrid ML is the mix of ML techniques, e.g., SL + UL; hybrid model ([Mustafee et al., 2020](#)) is combining a conventional one-approach simulation like DES or a hybrid simulation with either a single-approach ML model, or a hybrid ML.

We identified hybrid models that included hybrid simulation with RL/UL/SL ([Section 4.2.4](#)), hybrid ML with discrete simulation techniques ([Section 4.2.6](#)), and one study that included mixing a hybrid simulation consisting of ABS and DES with hybrid ML consisting of UL and SL ([Pereira et al., 2018](#)). In the last decade, hybrid simulation has emerged as a focal point of M&S research and practice ([Brailsford et al., 2019](#)). Thus, it is not surprising that we identified several studies that combined (predominantly) discrete techniques with ML approaches; however, there were only two hybrid simulation-ML studies that included optimization ([Behnamfar et al., 2022](#); [Pereira and Frazzon, 2021](#)). Considering the importance of optimal decision-making in supply chains, future research could explore the potential benefits and challenges of incorporating optimization into hybrid simulation-ML models.

Although hybrid ML techniques have been combined with discrete simulation methods, the number of such studies remains limited. Only two studies have combined hybrid ML with either DES ([Zhang et al., 2013](#)) or DES + ABS ([Pereira et al., 2018](#)), highlighting a significant gap in the literature. Combining ML with DES and ABS is particularly valuable because it leverages the strengths of both approaches: ML’s capability for pattern recognition, predictive analytics, and real-time data processing, alongside DES/ABS’s detailed modeling of stochastic processes. This synergy could lead to models that provide more accurate simulations of real-world systems by enhancing the precision of simulation parameters and also offer improved decision support by uncovering patterns and trends that might not be evident through traditional simulation analysis. Future research should, therefore, prioritize exploring this integration to fully realize its potential benefits in enhancing decision-making and operational efficiency in supply chains.

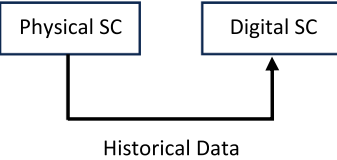
Our findings indicated the predominance of discrete simulation methods combined with ML, while SD was reported in fewer than ten studies ([Section 4.2.2](#)), highlighting a notable gap in the literature. Integrating SD models with ML offers several significant benefits. SD models are adept at capturing feedback loops and dynamic relationships within supply chain systems, but their accuracy heavily relies on the precision of their input parameters. ML can enhance SD models by improving the accuracy of these input parameters through its pattern recognition and predictive analytics capabilities. Moreover, ML can process and analyze real-time data related to the input parameters of SD models, enabling these models to continuously utilize the most current and relevant data. This dynamic adaptation supports more agile decision-making and ensures that the models accurately reflect the evolving nature of the system.

Furthermore, the integration of SD and ML holds substantial potential for streamlining policy interventions by predicting the outcomes of various strategies and identifying the most suitable interventions based

on historical data. The scalability and flexibility of ML complement the comprehensive perspective provided by SD models, facilitating the development of detailed and adaptable simulations. Future research should focus on advancing hybrid models that combine SD with ML,

investigating the most effective ML algorithms for enhancing SD models, and applying these integrated models to manage supply chain drivers more effectively. Additionally, it is crucial to assess the real-time performance of SD-ML models, explore their interpretability to ensure

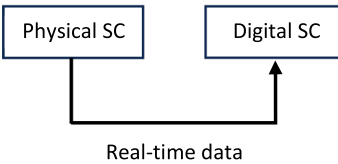
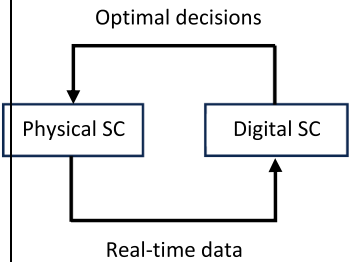
**Table 22**  
Subclasses of the Industry 4.0 Support Technologies.

Subclass	Data flow	Description	Publications
Digital model	 <pre> graph TD     Physical[Physical SC] --&gt; Digital[Digital SC]     Historical[Historical Data] --&gt; Digital             </pre>	Creating a SC model using historical data for analysis and decision-making.	Jacobson et al. (2021), Dahlem and Harrison (2010), Behnamfar et al. (2022), Raghuram et al. (2022), Jacobson et al. (2021), Bodendorf et al. (2022), Wang et al. (2022), Rana and Oliveira (2014), Karimi-Mamaghan et al. (2020), Afridi et al. (2020), Du and Xiao (2019), Priore et al. (2019), Lee and Sikora (2019), Mortazavi et al. (2015), Saitoh and Utani, (2013), Sui et al. (2010), Kim et al. (2010), Kwon et al. (2008), Jiang and Sheng (2009), Carbonneau et al. (2008), Li et al. (2008), Pan (2008), Chi et al. (2007), Zhang and Bhattacharyya (2007), Li and Zhao (2006), Pardoe and Stone (2005), Sheremetov et al. (2005), Ravulapati et al. (2004), Rao et al. (2003), Creighton and Nahavandi (2002), Idrees et al. (2006), Zhang et al. (2019), Okada et al. (2023), Walzberg et al. (2022), Esmaeili Avval et al. (2022), Kosasih and Brintrup (2022), El Shar et al. (2022), Etemadidavan and Collins (2022), Ktenioudaki et al. (2021), Sishi and Telukdarie (2021), Jackson and Velazquez-Martinez (2021), Hirano et

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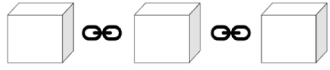
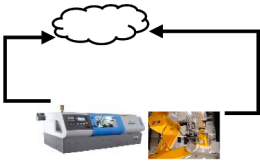


Table 22 (continued)

			<p>al. (2021), Barat et al. (2019a), Vondra et al. (2019), Yang et al. (2019), Aghaie and Hajian Heidary (2019), Barat et al. (2019b), Zhou et al. (2015), Yang and Zhang (2015), Tuncel et al. (2014), Zhang et al. (2013), Liu et al. (2011), Xu et al. (2009), Sheremetov and Rochamier (2008), Kaihara and Fujii (2008), Kiekintveld et al. (2007), Pardoe and Stone (2007), Kim et al. (2005), Pardoe and Stone (2004), Cao (2003), Kurian et al. (2023), Xiang (2020), Sankaran et al. (2022).</p>
<p>Digital shadow</p>		<p>Creating a SC model using real-time data for monitoring SC operations.</p>	<p>Wang et al. (2020)</p>
<p>Digital twin</p>		<p>Creating a SC model using real-time data for monitoring and controlling SC operations.</p>	<p>Emerson and Piramuthu (2004), Badakhshan and Ball (2023, 2024), Badakhshan et al. (2022), Serrano-Ruiz et al. (2022), Zou et al. (2022), Weihrauch et al. (2018), Bush et al. (2017), Lang et al. (2020), Waschneck et al. (2018), Gros et al. (2020), Yang et al. (2022), Mukherjee et al. (2022), Jaenichen et al. (2022), Greis et al. (2022), Corsini et al. (2022), Serrano-Ruiz et al. (2021), Shayeez and Panicker (2021), Gutierrez-Franco et al. (2021), Pereira and Frazzon (2021), Clark and Kulkarni (2021), Gružauskas et al.</p>

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Table 22 (continued)

			(2019), Zhou and Zhou (2019), Cavalcante et al. (2019), Ben Kacem et al. (2020), Pereira et al. (2018), Mehta and Yamparala (2014), Lin and Pai (2000), Lei et al. (2000a), Lei et al. (2000b), Schnieder et al. (2023), Hinde, and West (2023), Zdolsek Draksler et al. (2023), Guo et al. (2023)
Blockchain		Blockchain can enhance transparency, traceability, and efficiency in various stages of the SC.	Rooskhosh et al. (2023)
Cloud manufacturing		Cloud manufacturing is a model that leverages cloud computing technologies to provide on-demand manufacturing services.	Jinqi et al. (2017)

transparency and evaluate the computational efficiency of these hybrid models. Addressing these research areas will enable the field to leverage the combined strengths of SD and ML, resulting in more precise, adaptable, and insightful models for managing supply chains.

Another finding concerning SD is that it has not been integrated with RL (unlike DES and ABS). Integrating SD with RL offers significant benefits for enhancing the modeling and optimization of supply chains. SD excels at capturing feedback loops and dynamic interactions within systems, while RL is proficient at learning and adapting optimal policies through interaction with the environment. This integration allows for developing models that simulate dynamic supply chain behaviors and adapt and optimize SCM strategies. Future research should explore effective techniques for integrating SD with RL and apply these hybrid models to manage supply chain drivers more efficiently.

Despite its potential, the number of studies integrating Monte-Carlo simulations (MCS) with ML remains limited, with only eight studies identified (Section 4.2.3), indicating a notable gap in the literature. The benefits of integrating MCS with ML are substantial: ML can help refine the input distributions for MCS based on historical data, improving the reliability of the simulations. Furthermore, ML can identify complex relationships between variables that MCS might otherwise treat as independent, thereby enhancing the fidelity of the simulation outcomes. This integration can lead to more informed and robust decision-making, particularly in supply chains where uncertainty plays a critical role. Future research should focus on expanding the application of MCS-ML integration by exploring various ML algorithms that can effectively

complement MCS in addressing supply chain problems. Additionally, studies should assess the interpretability and transparency of the results generated by MCS-ML models to ensure that they are accurate and actionable for decision-makers.

5.3. Data flow mechanisms and cross-disciplinary research

To address RQ3, “What are the data flow mechanisms in hybrid models?”, we examined how data is exchanged among components in hybrid models. We identified four distinct Sim-ML classes related to data flow: sequential, feedback, sequential-feedback, and feedback-sequential. Brailsford et al. (2019) reviewed the literature on hybrid simulation and identified four forms of hybridization based on the level of interaction among the DES, ABS, and SD sub-models. Integration was the highest level of hybridization, where the sub-models became inseparable; the authors found only four studies that conformed to this definition (Brailsford et al., 2019). In our study, the hybrid models are a mix of simulation models and models developed using data-driven ML techniques. As such, there is no common frame of reference for simulated time (as with ABS, SD, and DES). Thus, it is arguable that seamless and inseparable integration (as per Brailsford et al., 2019) of M&S-ML hybrid models is not as common as in hybrid simulation studies.

The scope of the paper is on cross-disciplinary models, i.e., Hybrid Model Type D and E (Mustafee et al., 2020), and the discussion on sequential and feedback dataflow mechanisms helps us to present a critique of multidisciplinary, interdisciplinary, and transdisciplinary

research. In the paper on hybrid models and transdisciplinary research (Tolk et al., 2021), the authors identified sequencing of messages between discipline-specific models as one of the hallmarks of multidisciplinary research, integrability of models as an example of interdisciplinary research and composability of conceptualization allowing for the convergence of disciplines as transdisciplinary research. Our analysis of the data flow mechanisms revealed that the current state-of-the-art in M&S-ML is predominantly multidisciplinary, with both the M&S and the ML disciplines creating artifacts based on the extant knowledge constructs existing within disciplines; further, only through the exchange of information between the M&S and ML sub-models is hybridity achieved (Fig. 5; left). Future research direction can thus focus on the blending of disciplinary knowledge through interaction and integration, which will affect a shift towards interdisciplinary M&S-ML models (Fig. 5; center). Transdisciplinary research remains the final goal (Fig. 5; right), where the convergence of disciplinary knowledge may lead to new disciplines of study with hybridity as its core. They may develop novel methods and artifacts considered breakthroughs, coalescing the distinct identities of modeling approaches we now see in M&S and ML fields. These artifacts will no longer rely on data flow mechanisms since the new knowledge will have assimilated the existing scientific understanding from the M&S and ML fields, thereby creating a new field of study or a new discipline.

**Table 23**

Categorizing publications based on the five Sim-ML classes related to industrial sector criteria of Sim-ML.

Sim-ML Class	Sim-ML Subclass	Publications
Manufacturing	Electrical equipment	Roozkhosh et al. (2023)
	Basic metals	Liebenberg and Jarke (2023), Bodendorf et al. (2022)
	Transport equipment	Wang et al. (2022)
	Machinery and equipment	Karimi-Mamaghan et al. (2020)
	Computer, electronic, and optical products	Afridi et al. (2020), Lee and Sikora (2019), Weihrauch et al. (2018), Li et al. (2008), Pardoe and Stone (2004), Waschneck et al. (2018), Jaenichen et al. (2022)
	Food products	Zou et al. (2022), Rana and Oliveira (2014), Corsini et al. (2022), Ktenioudaki et al. (2021), Jackson et al. (2021), Gružauskas et al. (2019), Barat et al. (2019a) Okada et al. (2023)
	Pharmaceuticals, medicinal chemicals, and botanical products	
	Coke and refined petroleum products	Yanchun (2008)
	Motor vehicles, trailers, and semi-trailers	Gros et al. (2020)
	Fabricated metal products, except machinery and equipment	Cao (2003)
Other manufacturing	Raghuram et al. (2022), Walzberg et al. (2022)	
Transportation and storage	Postal and courier activities	Zdolsek Draksler et al. (2023), Schnieder et al. (2023)
Electricity, gas, steam, and air conditioning supply	Manufacture of gas; distribution of gaseous fuels through mains	Vondra et al. (2019)
Wholesale and retail trade	Retail trade, except for motor vehicles and motorcycles	Pereira and Frazzon (2021), Guo et al. (2023), Barat et al. (2019b), Pereira et al. (2018)
Human health and social work activities	Human health activities	Ben Kacem et al. (2020)

#### 5.4. Industry 4.0 technologies

To address RQ4, “How does hybrid modeling support the development of digital twins, which is an Industry 4.0 enabler?”, our Sim-ML literature classification framework includes digital models, digital shadows, and digital twins into the category of Industry 4.0 support technologies. Our review has also identified studies on blockchains and cloud manufacturing, both Industry 4.0 support technologies, and these have been included in our framework. A conventional M&S or ML model using historical data exemplifies a digital model. However, our review also includes Type E Hybrid models (Mustafee et al., 2020) that integrate M&S-ML models with real-time data sources and/or data acquisition technologies. Consequently, we have classified two additional subclasses, digital shadow, and digital twin, to represent hybrid models that incorporate real-time data.

Several studies developed conventional simulation models (digital models) or ML models trained on historical or synthetic data as proxies for real-time data and referred to them as digital twins. However, we accepted these claims due to the lack of a standardized definition of digital twins. From a disciplinary perspective, Mustafee et al. (2023) distinguish between digital models, real-time simulations (RtS), digital shadows, and digital twins. An RtS uses historical data combined with limited real-time data feeds, serving as an intermediary stage between a digital model that relies solely on historical data and fully developed digital shadows or digital twins that incorporate extensive real-time data feeds (ibid.). Future research on hybrid M&S-ML models in SCM should thus focus on methodological innovations to enable empirical SC modeling that integrates both historical and real-time data.

Our focus for the research question was on digital twins, and based on which a sub-set of database search terms were defined (Table 3). However, in our literature review, we identified two Industry 4.0 enablers that could be classified under support categories: Blockchain and Cloud Manufacturing. One study employed hybrid M&S-ML to predict blockchain acceptance rates in resilient supply chains (Roozkhosh et al., 2023). Another paper employed hybrid M&S-ML in an SC network in a cloud manufacturing environment (Jinqi et al., 2017). We critique the opportunities for using hybrid methods in relation to these Industry 4.0 enablers.

**Blockchain:** Hybrid M&S-ML approaches offer significant potential for advancing blockchain technology by providing a comprehensive analysis of blockchain systems. These approaches can simulate network performance, including transaction throughput and scalability, while ML can be applied to forecast future performance and optimize configurations. Additionally, ML can enhance blockchain security through anomaly detection and fraud prevention, with simulation models testing these algorithms under various scenarios. Furthermore, hybrid M&S-ML methods can refine consensus mechanisms and validate smart contracts through predictive analytics. Future research should focus on developing specific methodologies for integrating M&S-ML techniques with blockchain networks, exploring real-time anomaly detection and fraud prevention, optimizing consensus mechanisms, and assessing security risks. This comprehensive approach holds promise for improving blockchain technology in terms of performance, scalability, and security.

**Cloud manufacturing:** Hybrid M&S-ML can play a pivotal role in optimizing cloud manufacturing environments within supply chains by enabling real-time data processing, predictive analytics, and adaptive decision-making. In a cloud manufacturing setting, simulation models can be used to create digital representations of manufacturing processes and supply chain operations, while ML algorithms can analyze data from these simulations to predict outcomes, optimize resource allocation, and improve production scheduling. This integration allows for more efficient use of cloud-based resources, enhanced scalability, and the ability to respond dynamically to changes in demand or disruptions in the supply chain. Future research should focus on expanding the use of hybrid M&S-ML techniques in cloud manufacturing, particularly in

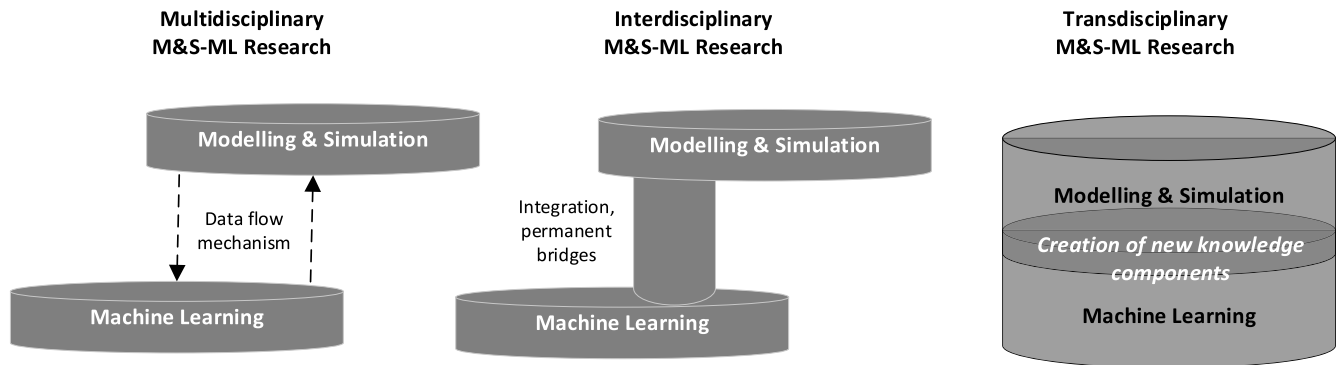


Fig. 5. Different forms of cross-disciplinary M&S-ML research (adapted from Tolk et al., 2021).

developing real-time adaptive models that can optimize complex supply chain networks in a cloud environment.

### 5.5. Industrial sectors

To address RQ5, “What is the extent of the adoption of hybrid modeling in addressing industrial use cases?”, we classified the papers according to the industrial sectors. Most studies present hybrid models for addressing problems in general supply chains; for example, the majority of the studies that we reviewed used simulation data to train ML algorithms. The lack of access to industrial data could be a reason for this. More industry-specific studies are needed. Thus, developing academic networks with industry partners will open up interesting real-world case studies in which a plethora of integrated M&S-ML models identified in this literature review could be applied based on various SCM contexts. This would go a long way in evidencing the efficacy of the hybrid M&S-ML modeling approach for SCM.

Our literature review makes several contributions. First, we recognize the increasing number of studies combining simulation methods with ML approaches in SCM, and we contribute to this growing area of research through a methodological review of papers. Second, we developed the *Sim-ML Literature Classification Framework* for literature synthesis. The framework builds on existing studies, e.g., [Chopra and Meindl \(2013\)](#) and [Mustafee et al. \(2020\)](#), with numerous additions made by the authors to capture the intricacies of the underlying literature. The hierarchical taxonomy consists of five SC criteria, 22 Sim-ML classes, and over 75 Sim-ML subclasses. Third, we identified the mix of the various M&S techniques used with supervised, unsupervised, and reinforcement learning. We also considered the mix of M&S-ML techniques with and without optimization. Fourth, we identified the various data flow mechanisms employed by the hybrid Sim-ML studies and categorized them into eight distinct data flow (DF) types – DF Types A-G. Finally, in the discussion section, we used the five SC criteria from our Sim-ML literature classification framework to discuss the avenues for future research. We hope the review will generate interest among the M&S community in mixing methods that go wider than hybrid simulation and where data-driven/ML approaches are combined with M&S, thereby affecting a shift from hybrid simulation to hybrid modeling ([Mustafee and Powell, 2018](#)). Our review is also a key source of information for the ML community, which may see the promise of using M&S to supplement ML approaches currently used for SCM analysis.

### 5.6. Practical implications

The integration of M&S with ML offers substantial benefits for supply chain practitioners, providing a powerful toolset to address complex and dynamic supply chain challenges. By leveraging the strengths of both approaches, i.e., simulation’s ability to model intricate system dynamics and ML’s capacity for clustering and predictive analytics, practitioners can achieve more accurate, data-driven decision-making.

Hybrid M&S-ML models empower practitioners to simulate “what-if” scenarios and harness ML to provide actionable insights. Simulation explores different strategies based on predefined scenarios, while ML learns from historical and real-time data to enhance predictions and guide SCM policies. This combined approach is particularly useful for managing supply chain drivers like inventory, sustainability, and sourcing, ensuring more precise and effective decision-making. For instance, hybrid M&S-ML models can simulate the environmental impact of various supply chain practices and policies and help design strategies to minimize carbon footprints.

Hybrid M&S-ML models are crucial in mitigating the risks associated with supply chain disruptions. Simulation models the effects of various disruptions, allowing practitioners to explore a range of scenarios and assess their potential impacts on the supply chain. ML enhances this process by predicting the likelihood of these disruptions based on historical and real-time data, enabling more accurate risk assessments. Together, these methods allow for the development of more robust contingency plans, significantly enhancing the resilience of the supply chain.

The dynamic nature of supply chains requires continuous monitoring and adaptation. Hybrid M&S-ML models can incorporate real-time data to adjust strategies as conditions change, ensuring supply chain operations remain efficient and responsive. This real-time adaptation is crucial in industries such as retail and manufacturing, where demand patterns and supply conditions are volatile. For instance, in the retail sector, hybrid M&S-ML models can assist in managing inventory levels dynamically based on current sales trends and supply chain disruptions. In manufacturing, these models can adjust production and transportation schedules to address changes in demand or supply constraints effectively.

As supply chains evolve with the adoption of Industry 4.0 technologies, hybrid M&S-ML models can significantly enhance the integration of emerging technologies such as digital twins, blockchain and cloud manufacturing. ML plays a crucial role in this process by analyzing vast amounts of real-time data generated by these technologies. Based on this data it can identify patterns, predict system performance, and refine decision-making. While simulation helps understand the interactions and potential impacts of these technologies within supply chain processes, ML adds the ability to continuously learn from new data, refine predictions, and adapt strategies dynamically. This combined approach allows managers to simulate, predict, and streamline the implementation and scaling of new innovations, ensuring that they are effectively integrated into existing supply chain operations.

Based on the learnings from the literature and our modelling experience, we offer practitioners a set of guidelines to effectively implement hybrid M&S-ML models in SCM. First, we consider the involvement of stakeholders is necessary to define clear objectives and the scope of the hybrid models. In the SCM context, the objectives should focus on specific supply chain drivers such as inventory and transportation. Assessment of data requirements is essential to ensure relevant historical and



real-time data is available for simulation and ML components of the hybrid models. Development of a conceptual model can help with the selecting the correct mix of hybrid methods; additionally, model conceptualisation exercise may reveal that a hybrid solution is not necessary since the modelling objectives could be realised through either a simulation or a ML-based approach. For solutions that would benefit from hybrid Sim-ML approach, the selection of right tools and technologies is crucial, with Python being a popular choice due to its extensive libraries. Python's libraries, including *SimPy*, *AgentPy*, and *PySD* for simulation, and *Scikit-learn*, *TensorFlow*, and *PyTorch* for ML, support seamless integration. Subsequent to the selection of the tools, practitioners can consider connecting hybrid Sim-ML models to existing systems such as ERP and CRM to ensure secure and consistent data flows. Such IT-systems integration would enable the implementing of real-time data feeds through data pipelines and enable regular model updates. The models must undergo rigorous validation and testing for accuracy, followed by stakeholder training. Lastly, ongoing monitoring and adjustments are necessary to maintain performance, with clear documentation and communication of results to stakeholders.

In summary, supply chain practitioners stand to benefit significantly from the adoption of hybrid M&S-ML techniques. These models provide them with comprehensive analytical means for addressing the pressing challenges of modern supply chains, from improving operational efficiency and resilience to fostering innovation and real-time adaptability. As the supply chain environment continues to evolve, hybrid M&S-ML will become increasingly vital in achieving competitive advantage and operational excellence.

#### CRedit authorship contribution statement

**Ehsan Badakhshan:** Writing – original draft, Methodology, Investigation, Data curation, Conceptualization. **Navonil Mustafee:** Writing – original draft, Methodology, Investigation. **Ramin Bahadori:** Writing – review & editing, Methodology, Investigation.

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#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

#### Data availability

Data will be made available on request.

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