Integration of System Dynamics and Machine Learning: A Comprehensive Literature Review

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Abstract

This literature review examines the emerging field of integrating System Dynamics (SD) and Machine Learning (ML) methodologies, synthesizing findings from 58 highly relevant studies published between 2001 and 2026. The integration of these paradigms addresses fundamental challenges in modeling complex systems: SD provides causal structure and theoretical grounding for long-term policy analysis, while ML offers data-driven pattern recognition and predictive capabilities. This review identifies four primary integration approaches: (1) ML-based parameter estimation for SD models, (2) ML-driven policy optimization and control, (3) hybrid simulation frameworks combining SD structure with ML components, and (4) data-driven structure learning for SD models. Applications span public health, supply chain management, energy systems, manufacturing, and environmental sustainability. Despite significant methodological advances, critical research gaps persist in theoretical frameworks for integration, scalability to large-scale systems, validation methodologies, and standardized computational tools. These gaps present substantial opportunities for advancing both theoretical understanding and practical implementation of hybrid SD-ML systems.

Keywords: System dynamics; Machine learning; Hybrid simulation modeling; Parameter estimation; Policy optimization; Systematic literature review; Uncertainty quantification.

1. Introduction

System Dynamics (SD) and Machine Learning (ML) represent two fundamentally different yet potentially complementary approaches to understanding and modeling complex systems. System Dynamics, pioneered by Jay Forrester in the 1950s, emphasizes causal relationships, feedback loops, and stock-flow structures to capture the endogenous behavior of systems over time (Schwaninger, 2006). Machine Learning, rooted in statistical learning theory and computational intelligence, excels at discovering patterns in data and making predictions without explicit programming of causal relationships. The integration of these paradigms has emerged as a promising research frontier, motivated by the limitations inherent in each approach when applied independently. Traditional SD modeling faces significant challenges in parameter estimation, particularly for complex models with numerous parameters and limited historical data (Gadewadikar et al., 2023). Conversely, pure ML approaches often lack interpretability and struggle to capture the causal mechanisms and feedback structures that drive system behavior over extended time horizons (Abdelbari et al., 2017). The integration of SD and ML seeks to leverage the strengths of both methodologies: SD's ability to encode domain knowledge and causal structure, combined with ML's capacity for data-driven learning and pattern recognition (Rahmandad et al., 2025).

This literature review synthesizes research on SD-ML integration published over the past two decades, with particular emphasis on recent advances from 2001–2026. To ensure comprehensive coverage, particularly in rapidly expanding domains such as environmental management, this study cross-

references recent domain-specific reviews (e.g., Nesanır et al., 2025), thereby expanding the foundational synthesis to encompass a broader range of recent state-of-the-art applications. The temporal distribution of the reviewed literature highlights a significant acceleration in this research intersection, particularly post-2020. As illustrated in Figure 1, while early foundational works appeared in the 2000s, the application of machine learning within system dynamics models has experienced exponential growth in the current decade.

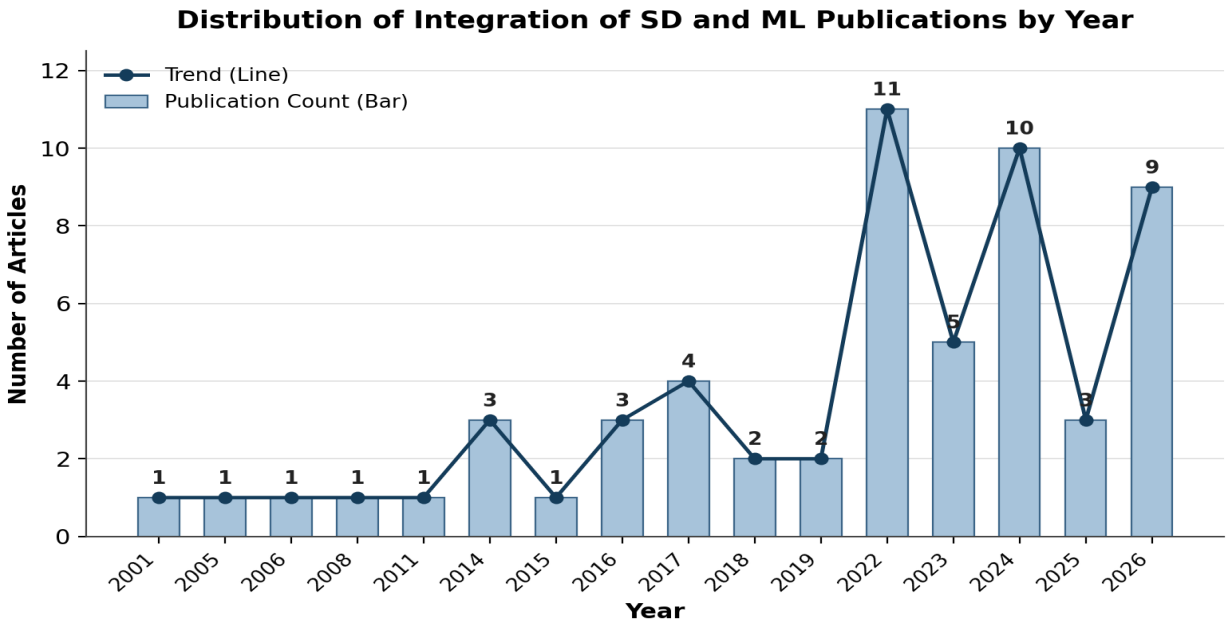

Figure 1. Distribution of integration of SD and ML publications by year.

Indeed, this momentum has carried into the current year: a further cluster of 2026 studies extends hybrid SD-ML modeling into new application domains and a widening set of contributing countries. This rapid upward trend underscores the increasing recognition of hybrid modeling as a critical and timely tool for addressing complex, data-rich systemic challenges. The review addresses five key questions: (1) What methodological approaches have been developed for integrating SD and ML? (2) In which application domains has SD-ML integration demonstrated value? (3) What theoretical frameworks guide the integration of these paradigms? (4) What are the current state-of-the-art techniques and their limitations? (5) What critical research gaps remain to be addressed? By answering these questions, this review provides a comprehensive foundation for future research and identifies specific opportunities for methodological innovation.

1.1 Review Methodology and Search Strategy

This review followed a structured, PRISMA-based protocol to identify, screen and synthesize the literature on the integration of System Dynamics (SD) and Machine Learning (ML). Consistent with recent systematic reviews of SD–ML and SD–AI integration, the search combined a primary bibliographic database (Scopus) with two complementary sources — Google Scholar (to capture highly cited and grey literature) and arXiv (to capture recent pre-prints in fast-moving ML sub-fields). The search window spanned 2001–2026 and was restricted to English-language records.

Search queries were constructed around three conceptual building blocks — System Dynamics terms, Machine Learning / AI methods, and integration / linkage terms — combined with Boolean AND across

blocks and OR within each block. Figure 2 presents these building blocks, and Table 1 lists the exact query strings executed in each database.

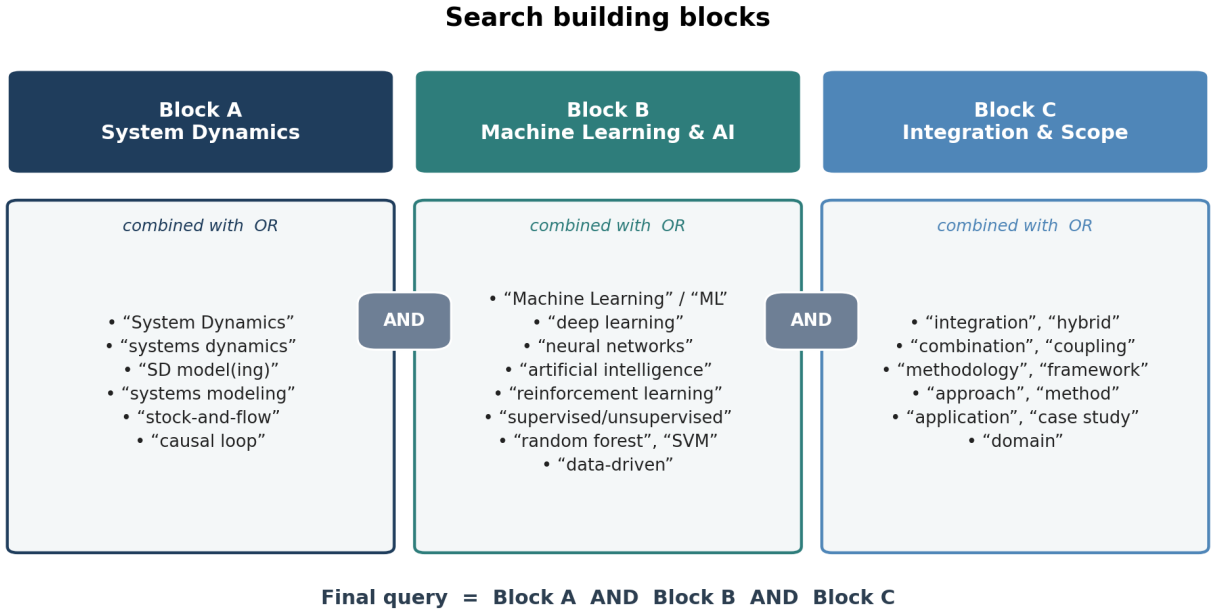

Figure 2. Search building blocks. Terms within a block were combined with OR; the three blocks were combined with AND (Block A AND Block B AND Block C).

The resulting database-specific query strings are reported in Table 1.

Database	Query string
Scopus (primary)	TITLE-ABS-KEY((“System Dynamics” OR “SD model*”) AND (“Machine Learning” OR “deep learning” OR “neural network*” OR “reinforcement learning” OR “artificial intelligence”) AND (“integrat*” OR “hybrid” OR “coupl*” OR “data-driven”)) — LIMIT-TO(LANGUAGE,“English”)
Google Scholar #1	((“System Dynamics” OR “systems dynamics” OR “SD modeling”) AND (“Machine Learning” OR “deep learning” OR “neural networks” OR “artificial intelligence”) AND (“integration” OR “hybrid” OR “combination” OR “coupling”))
Google Scholar #2	((“System Dynamics” OR “SD model”) AND (“ML” OR “machine learning” OR “data-driven”) AND (“methodology” OR “framework” OR “approach” OR “method”))
Google Scholar #3	((“System Dynamics” OR “systems modeling”) AND (“reinforcement learning” OR “supervised learning” OR “unsupervised learning”) AND (“application” OR “case study” OR “domain”))
arXiv #1	all:system+dynamics+AND+machine+learning+integration
arXiv #2	all:system+dynamics+AND+deep+learning+hybrid+model
arXiv #3	all:systems+modeling+AND+neural+networks+data-driven

Table 1. Exact search strings executed in each database (search window 2001–2026; English only).

Figure 3 summarizes the volume of records retrieved from each database and the subsequent screening funnel: a total of 1,058 records were retrieved and reduced to 290 unique records after de-duplication, of which 30 met the inclusion criterion in full-text assessment.

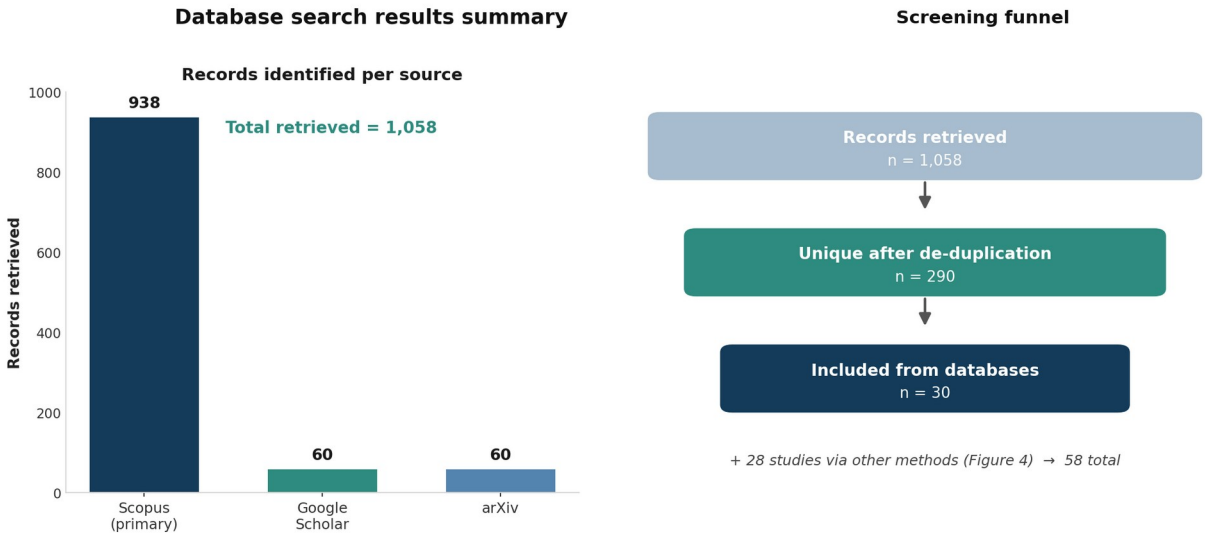

Figure 3. Database search results summary: records identified per source and the screening funnel (1,058 retrieved → 290 unique → 30 included from databases). A further 28 studies were identified via other methods (Figure 4), giving 58 in total.

The complete screening and selection process is summarized in the two-arm PRISMA 2020 flow diagram in Figure 4. In the database-search arm, records were de-duplicated, screened by title and abstract, and assessed in full text against the inclusion criterion of an explicit, operational integration of SD and ML; literature reviews, studies treating only SD's impact on AI (rather than integration), conference review items, and non-English records were excluded, leaving 30 included studies. A second arm identified studies through other methods — citation searching of a recent domain-specific review (Nesanır et al., 2025) together with manual and expert additions, including seven 2026 studies — contributing 28 further studies, so that the two arms together yield the 58 studies synthesized in this review.

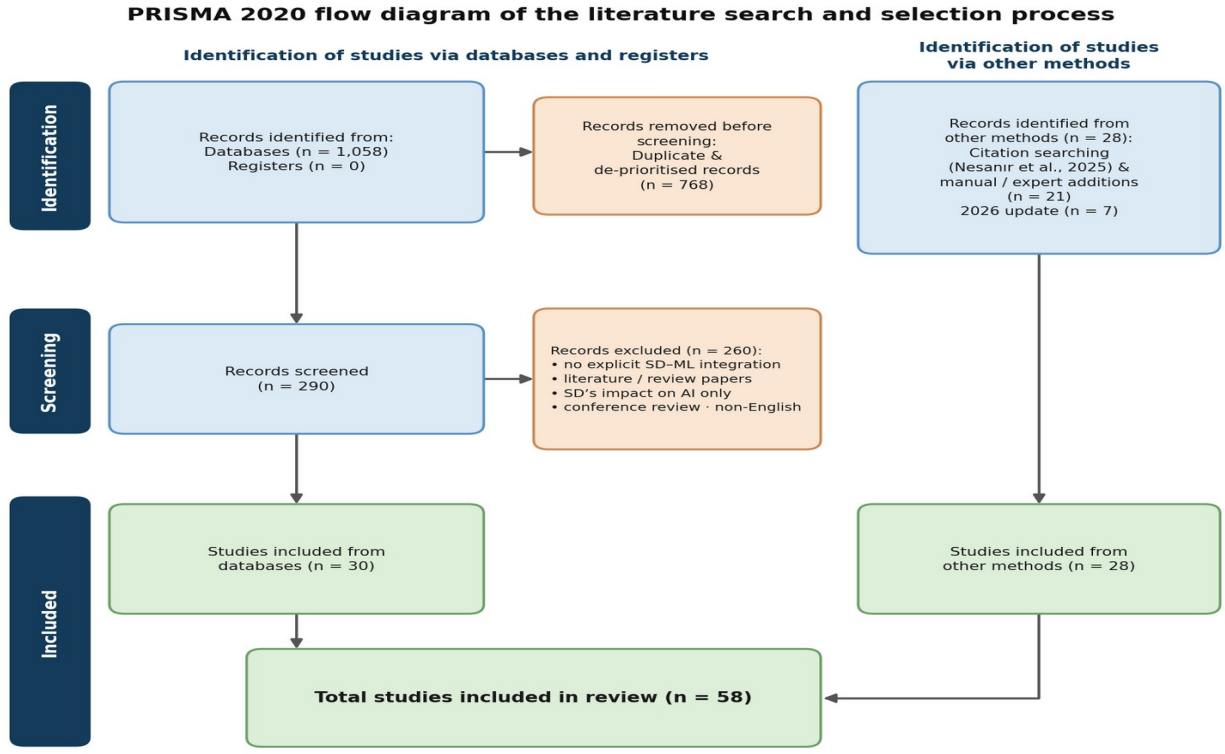

Figure 4. PRISMA 2020 flow diagram of the literature search and selection process (58 studies included: 30 via database searching and registers, 28 via other methods).

1.2 Geographic and Institutional Distribution of Research

The global interest in SD-ML integration is reflected in the geographic diversity of the contributing institutions and the locations of the case studies analyzed. A detailed institutional and geographic mapping of the reviewed literature reveals prominent research hubs. Figure 5 visualizes this distribution as a bar chart, in which each bar's length is proportional to the number of contributing papers in the reviewed corpus. As the visualization indicates, researchers from institutions in the United States, Iran, and China demonstrate a dominant presence in this field, with Taiwan and India also contributing multiple studies. Notably, the most recent wave of research has broadened the geographic base of the field: contributions from China and India have continued to grow, and new entrants — including Slovenia, Romania, Mexico, Belgium, and Nigeria — appear among the 2026 studies, reflecting the increasingly global diffusion of hybrid SD-ML modeling across diverse regional, industrial, and environmental contexts.

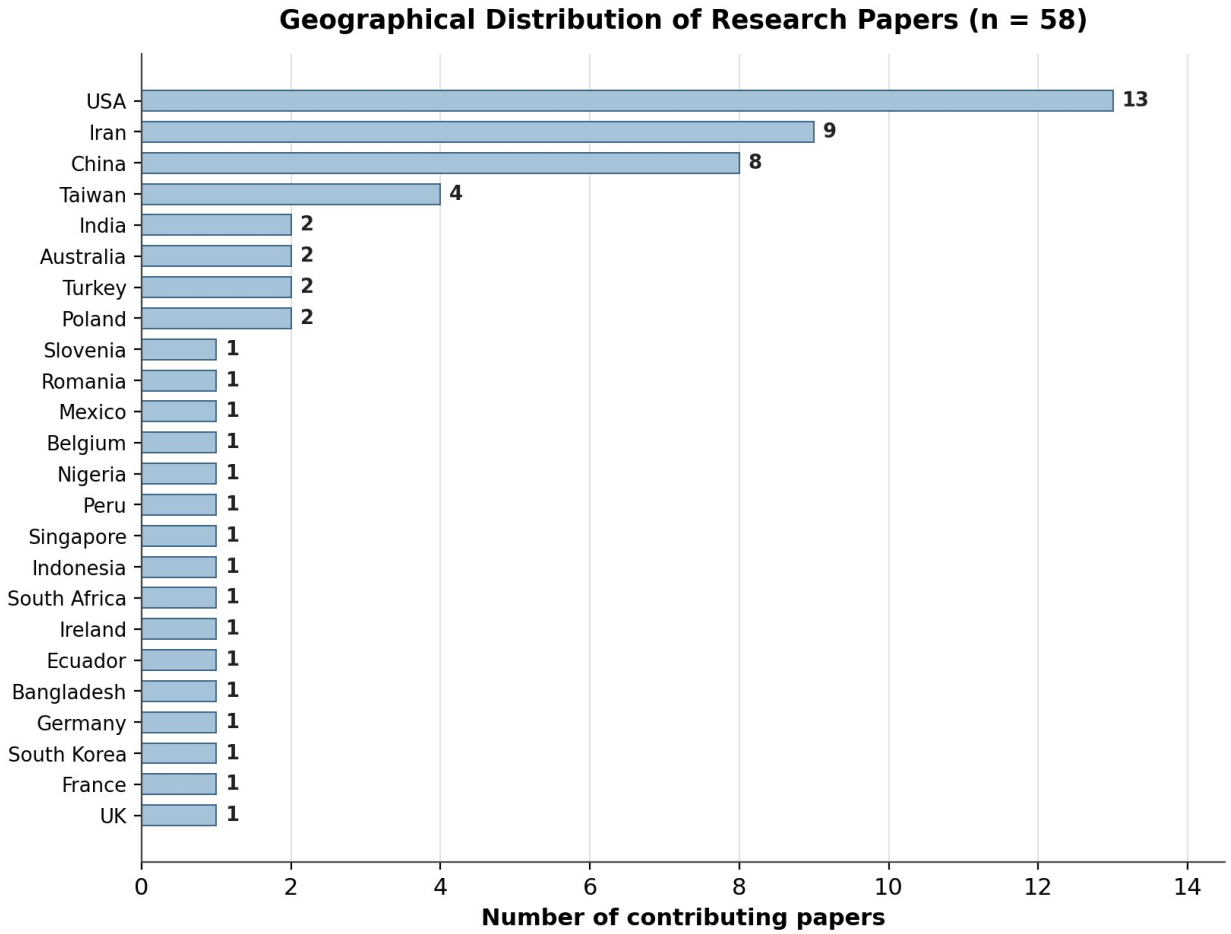

Figure 5. Geographical distribution of research papers (n = 58; bar length is proportional to the number of contributing papers in the reviewed corpus).

The literature reveals four primary methodological approaches for integrating System Dynamics and Machine Learning, each addressing different aspects of the modeling process and offering distinct advantages and limitations. A quantitative breakdown of the reviewed literature shows that hybrid simulation frameworks are the most common approach (37 of 58 studies, 63.8%), followed by ML-driven policy optimization and control (9 studies, 15.5%), data-driven structure learning (7 studies, 12.1%), and ML-based parameter estimation (5 studies, 8.6%). As shown in Figure 6, while the theoretical possibilities are vast, researchers most commonly adopt hybrid simulation structures, although policy-optimization and structure-learning approaches together account for a sizeable share of the field.

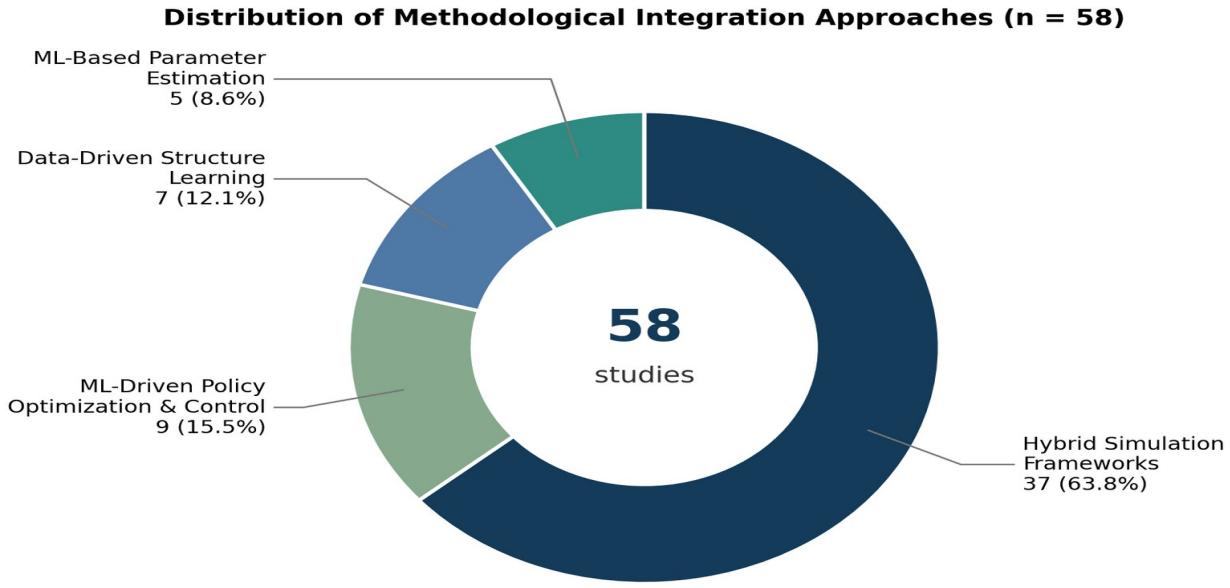

Figure 6. Distribution of methodological integration approaches.

Beyond the geographic spread, the field's intellectual structure is shaped by distinct networks of researchers driving specific thematic clusters. Mapping prominent author groups onto their primary methodological focus and the application domains they engage reveals the structural landscape of the

field (Figure 7).

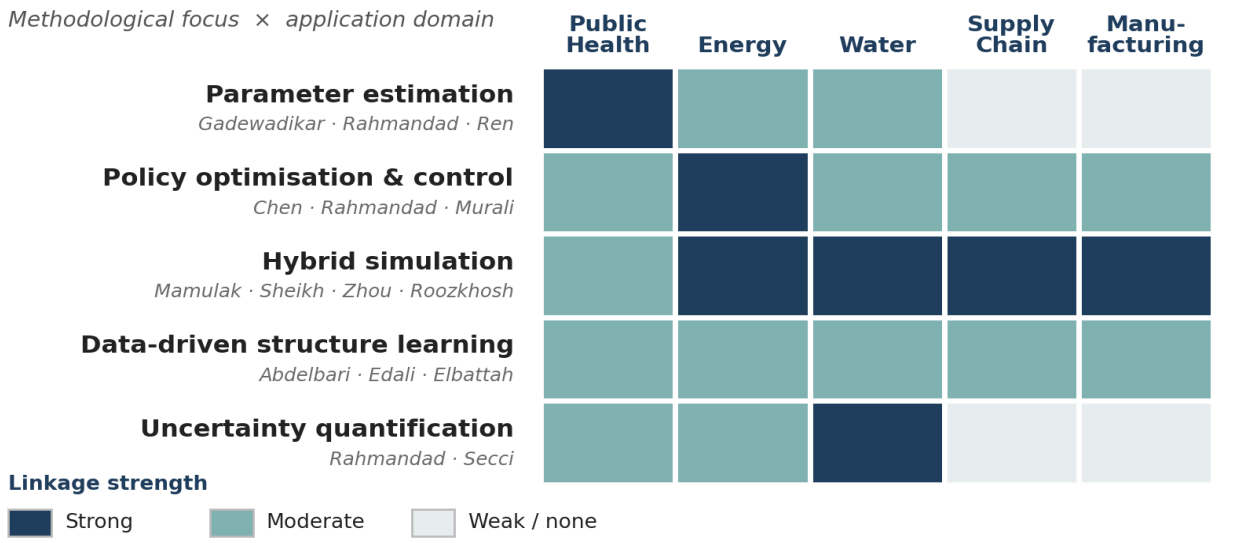

Figure 7. Author–Focus–Domain linkage matrix. Cell shading denotes the strength of research activity linking each methodological focus (and its representative authors) to an application domain: dark navy = strong, teal = moderate, light = weak/none.

The linkage matrix demonstrates cross-pollination between specific methodological developments and practical domains. For instance, work on parameter estimation is tightly linked to public health, driven by the immediate data needs of pandemic modeling. Conversely, hybrid simulation serves as a central hub bridging highly diverse sectors, from energy systems to water resources. Identifying these clusters highlights the current centers of gravity in the literature and points to isolated domains where future interdisciplinary collaboration is needed.

2. Theoretical Foundations and Conceptual Framework

2.1 Complementary Paradigms

The theoretical rationale for integrating System Dynamics and Machine Learning rests on the complementary nature of these paradigms. System Dynamics is grounded in control theory, feedback systems, and causal loop thinking, emphasizing the endogenous generation of system behavior through feedback mechanisms and accumulation processes (Schwaninger, 2006). This approach excels at capturing qualitative system structure and testing policy interventions, but traditionally relies on expert judgment for parameter specification and model structure determination.

Machine Learning, by contrast, is rooted in statistical learning theory, optimization, and pattern recognition. ML algorithms excel at discovering complex nonlinear relationships in high-dimensional data spaces and making accurate predictions, but typically operate as “black boxes” with limited interpretability and no explicit representation of causal mechanisms (Elbattah et al., 2017). The integration of these paradigms can potentially overcome the limitations of each: SD provides the causal scaffolding and theoretical coherence, while ML contributes data-driven parameter estimation, pattern discovery, and enhanced predictive accuracy (Kamdem, 2024).

2.2 Theoretical Integration Frameworks

Several theoretical frameworks have been proposed to guide SD-ML integration. Schwaninger (2006) discusses the potential for combining SD with neural networks, control theory, and agent-based modeling, positioning SD within the broader systems movement and identifying complementarities with computational intelligence approaches. However, this early work lacks concrete integration methodologies and remains largely conceptual.

More recently, Kamdem (2024) proposes a framework for integrating machine learning with causal inference to enhance system dynamics modeling, emphasizing the prediction of complex interactions. This framework attempts to bridge the gap between correlation-based ML predictions and causation-based SD modeling, though practical implementation details remain limited. The theoretical challenge lies in reconciling the fundamentally different epistemological foundations: SD's emphasis on understanding causal mechanisms versus ML's focus on predictive accuracy (Abdelbari et al., 2017).

2.3 Hybrid Modeling Paradigms

The concept of hybrid modeling—combining mechanistic (theory-driven) and empirical (data-driven) approaches—provides a broader theoretical context for SD-ML integration. Shekhar et al. (2023) develop a hybrid mechanistic-machine learning approach for modeling industrial network dynamics, demonstrating how mechanistic SD models can be augmented with ML components to capture phenomena that are difficult to model from first principles. This hybrid paradigm recognizes that real-world systems often contain both well-understood causal mechanisms (suitable for SD representation) and complex, data-rich phenomena (suitable for ML modeling) (Timma et al., 2015).

Timma et al. (2015) explore hybrid modeling practices for technological substitution, combining SD with other computational methods. These works highlight the methodological flexibility required when integrating different modeling paradigms and the importance of clearly delineating which aspects of system behavior are captured by each component of the hybrid model.

3. Methodological Integration Approaches

As shown earlier in Figure 6 (Section 1.2), the prevalence of Hybrid Simulation Frameworks suggests that practitioners currently find the most practical value in maintaining SD and ML as distinct but interacting modules. Meanwhile, Data-Driven Structure Learning remains a niche but highly promising frontier. The following subsections detail the mechanics, advantages, and limitations of each of these four primary methodologies. These categories reflect the primary role played by machine learning in each study; accordingly, SD–ML studies whose ML component mainly performs parameter estimation, policy optimization, or structure learning are assigned to those categories rather than to Hybrid Simulation Frameworks, which is reserved for studies in which SD and ML operate as coupled predictive components.

3.1 ML-Based Parameter Estimation

The most prevalent integration approach uses machine learning algorithms to estimate parameters for system dynamics models, addressing one of SD's most significant practical challenges. Gadewadikar et al. (2023) present a comprehensive methodology incorporating regression-based AI (support vector machines, artificial neural networks, and random forests) into SD models for parameter estimation. Their approach creates an integrated environment where model parameters can be continuously updated with new data while maintaining model integrity. Applied to a susceptible-infected-recovered (SIR) model with COVID-19 data, this methodology demonstrates how AI can enhance the efficiency and data-responsiveness of SD models.

Rahmandad et al. (2025) advance this approach significantly by incorporating deep learning into system dynamics through amortized Bayesian inference for scalable likelihood-free parameter estimation. Their neural posterior estimation technique enables instant generation of parameter posteriors for complex SD models, overcoming the computational bottlenecks of traditional Bayesian calibration methods. Applied to an epidemiological SEIRb model, this approach achieves orders-of-magnitude speedup in parameter estimation while providing full posterior distributions that quantify uncertainty. The methodology represents a significant advance in making Bayesian inference practical for complex SD models, though it requires substantial upfront computational investment to train the neural networks.

Ren et al. (2005) and Alborzi (2006) explore earlier approaches to parameter estimation using artificial neural networks, demonstrating the long-standing interest in this integration strategy. These works establish foundational concepts for using ANNs to capture complex nonlinear relationships that are difficult to specify analytically in SD models, though they lack the sophisticated inference frameworks of more recent approaches.

A closer reading of these studies shows that the parameters targeted by machine learning are overwhelmingly the dynamic rate constants and behavioral-response coefficients that SD modelers have traditionally fixed by expert judgment. In the epidemiological applications that dominate this strand, the estimated quantities are the transmission (infection) rate β, the incubation or latency rate, and the recovery rate γ — together with the implied basic reproduction number R_0. Rahmandad et al. (2025) extend this set, inferring behavioral contact-reduction coefficients, vaccine effectiveness, immunity-loss time and the infection-fatality rate among the twelve parameters of their SEIRb model. Beyond epidemiology, the same logic is applied to adoption- and demand-response rates (Roozkhosh et al., 2022; Mamulak et al., 2024) and, in the tightest couplings, to structural and policy parameters that are co-evolved with the model structure itself (Chen et al., 2011). Table 2 summarizes the specific parameters estimated in the principal studies.

Study	ML method	Target SD model	Parameters estimated
Gadewadikar et al. (2023)	SVM, ANN, random forest (regression AI)	SIR (COVID-19)	Transmission rate β, recovery rate γ, implied R_0
Rahmandad et al. (2025)	Deep learning – amortized Bayesian inference (neural posterior estimation)	SEIRb (+ Random Walk)	Transmission, incubation/latency and recovery rates; behavioral contact-reduction; vaccine effectiveness; immunity-loss time; infection-fatality rate (12 parameters)
Ren et al. (2005); Alborzi (2006)	Artificial neural networks	Generic nonlinear SD	Nonlinear functional / rate parameters hard to specify analytically
Chen et al. (2011)	Recurrent neural networks	Policy-design SD	Structural and policy parameters co-evolved to fit a reference mode
Roozkhosh et al. (2022)	MLP + support-vector regression	Blockchain-adoption SD	Adoption / acceptance-rate parameters
Mamulak et al. (2024)	Random forest	Sales-forecasting SD	Demand / sales-response parameters

Table 2. Types of parameters estimated by ML in the principal SD–ML parameter-estimation studies.

3.2 ML-Driven Policy Optimization and Control

A second major integration approach employs machine learning for policy optimization and control within SD models. Chen et al. (2011) propose a policy design method using recurrent neural networks (RNNs) that simultaneously evolves both system structure and parameter values to fit a desired reference mode. This approach represents a tight coupling of SD and ML, where the neural network not only optimizes parameters but also explores alternative model structures. The methodology allows policymakers to specify desired system behavior and automatically discover policies that achieve those outcomes, though it lacks concrete domain applications and raises questions about the interpretability of automatically generated model structures.

Rahmandad et al. (2008) explore learning control policies in system dynamics models, extending the application of ML beyond parameter estimation to the discovery of effective intervention strategies. This work addresses the challenge of policy design in complex systems where the optimal intervention strategy may be non-obvious and context-dependent. By using ML to learn control policies directly from simulation data, this approach can discover sophisticated, adaptive policies that outperform simple rule-based interventions.

Murali et al. (2024) demonstrate hybrid simulation with reinforcement learning-based scheduling for resilient infrastructure networks, showing how RL can optimize operational decisions within an SD framework. This application illustrates the potential for ML-driven control in real-time operational contexts, though the integration between SD and RL components remains relatively loose, with SD primarily providing the simulation environment for RL training.

3.3 Hybrid Simulation Frameworks

A third integration approach develops hybrid simulation frameworks that combine SD structure with ML components for specific modeling tasks. Mamulak et al. (2024) integrate system dynamics with random forest algorithms for sales forecasting, demonstrating how ML can enhance the predictive accuracy of SD models in business applications. The random forest component captures complex nonlinear patterns in sales data that would be difficult to model explicitly in SD, while the SD framework maintains the causal structure and feedback mechanisms driving market dynamics.

Sheikh et al. (2025) develop a system dynamics and machine learning approach for optimizing semiconductor manufacturing in small and medium enterprises. Their hybrid framework uses SD to model production flows and capacity dynamics while employing ML for demand forecasting and quality prediction. This work demonstrates the practical value of hybrid approaches in manufacturing contexts, though the integration methodology remains domain-specific and may not generalize easily to other applications.

Zhou et al. (2024) present an intelligent framework for optimizing water-energy-food nexus synergies in urban metabolic landscapes, combining SD with machine learning for sustainability analysis. This application illustrates how hybrid frameworks can address multi-objective optimization problems in complex socio-technical systems, using SD to capture long-term dynamics and feedback effects while ML handles pattern recognition in high-dimensional sustainability indicator spaces.

Roozkhosh et al. (2022) develop a hybrid system dynamics and machine learning approach for predicting blockchain acceptance rates in resilient supply chains. Their methodology uses SD to simulate adoption dynamics and then feeds simulation results into multilayer perceptron (MLP) and support vector regression (SVR) models for prediction. This sequential integration approach demonstrates one pattern for combining SD and ML, though the coupling remains relatively loose with limited bidirectional interaction between components.

Recent methodological advancements have expanded hybrid frameworks to incorporate complex spatial, physical, and climate models alongside SD and ML. For instance, Secci et al. (2024) propose a highly integrative methodology for groundwater management that combines process-based physical models, data-driven ML algorithms, and SD, highlighting the interdependence and complementarity of these diverse paradigms. Similarly, Rahmani et al. (2015) successfully merged statistical weather generators with hybrid data-driven and SD models to account for complex climatic uncertainties. Advancing multi-dimensional nexus modeling, Chang et al. (2026) developed an extensive framework integrating SD and ML to establish a Water-Energy-Food-Climate-Land (WEFCL) nexus for aquavoltaics, extending the scope of traditional multi-objective optimization. Furthermore, Zhang et al. (2024) demonstrated the fusion of Land Change Models with SD and ML to simulate and predict ecosystem carbon sequestration under various climate scenarios, demonstrating that hybrid frameworks can effectively bridge spatial modeling with temporal system dynamics.

Borlinič Gačnik et al. (2026) integrate machine learning with system dynamics for climate-resilient viticulture, combining multivariate temperature-trend analysis and several ML regressors (random forest, support vector machines, decision trees, and linear regression) with a stock-and-flow SD model of vineyard biomass growth. While the ML models identify the dominant predictors of wine quality, the SD component simulates nonlinear growth responses, feedback effects, and carrying-capacity constraints, revealing threshold behavior with optimal biomass near 25 °C and a sharp decline beyond heat-stress thresholds. The study illustrates how a hybrid framework can bridge ML-based prediction with SD-based explanation for long-term climate-adaptation planning.

Jia & Zhang (2026) propose an integrated machine-learning–system-dynamics–optimization framework for land–water allocation under climate change, in which ML models generate long-horizon daily climate sequences that drive an SD model of soil moisture, yield formation, basin-scale allocable water, and farm returns, while a non-dominated sorting genetic algorithm (NSGA-II) searches Pareto-optimal cropping and irrigation strategies. Applied to a rice–wheat system in the middle Yangtze River Basin, the framework raises irrigation water productivity while maintaining near-baseline profits and exposes a scarcity-regime threshold beyond which economic policy instruments become second-order to binding biophysical constraints. The work exemplifies the tight coupling of SD with both data-driven and optimization components for policy trade-off analysis.

Paul et al. (2026) develop a hybrid system-dynamics–machine-learning method for sustainable vehicular transport, simulating the dynamic interactions among product demand, travel distance, fuel price, and vehicle characteristics with an SD model and employing ensemble learning across four ML algorithms to improve predictive accuracy. Sobol sensitivity analysis and five scenario analyses identify fuel price, vehicle speed, and product demand as the most influential drivers of system adaptability, demonstrating how ML can sharpen the predictive layer of an SD sustainability model under uncertainty.

Lazăr et al. (2026) combine random forest analysis, satellite remote sensing, and system dynamics to assess and mitigate eutrophication in the Romanian Black Sea coastal zone. Random forest identifies dissolved inorganic nitrogen, phosphate, salinity, and temperature as the dominant predictors of chlorophyll-a, while an SD model simulates ecosystem responses under nutrient-reduction, grazing-restoration, and combined management scenarios; the combined-intervention scenario achieves the strongest modeled reduction in chlorophyll-a, providing a scenario-based decision-support tool for ecosystem-based marine management.

De-la-Cruz-Madrigal et al. (2026) present an intelligent decision-support system that couples system-dynamics modeling with deep learning for the detection of risk and disruption in supply chains. The SD model captures the structural feedback and propagation dynamics of disruptions, while the deep-

learning component provides predictive detection, illustrating how hybrid SD–ML architectures can support proactive rather than reactive supply-chain risk management.

Extending hybrid SD–ML approaches into safety-critical engineering, Udu & Okpala (2026) propose a data-driven and predictive framework for engineering safety in complex systems that integrates machine learning, human-factors analysis, and system dynamics. The SD component represents the feedback structure linking technical, organizational, and human factors that shape safety performance, while the ML component provides predictive assessment of safety outcomes, illustrating how coupled SD–ML architectures can support proactive safety management.

3.4 Data-Driven Structure Learning

The fourth integration approach uses machine learning to learn system structure from data, potentially automating or augmenting the traditional SD model-building process. Abdelbari et al. (2017) develop a computational intelligence-based method to learn causal loop diagram-like structures from observed data. This approach addresses a fundamental challenge in SD modeling: the reliance on expert judgment for identifying feedback loops and causal relationships. By using ML to discover structure from data, this methodology could make SD modeling more accessible and data-driven, though significant challenges remain in ensuring that discovered structures are causally valid rather than merely correlational.

Edali (2022) proposes pattern-oriented analysis of system dynamics models via random forests, using ML to analyze and understand the behavior of existing SD models. This approach employs random forests to identify which parameters and structural features most strongly influence model behavior, providing insights that can guide model refinement and policy design. While not directly integrating ML into the SD model itself, this methodology demonstrates how ML can enhance the analysis and interpretation of SD models.

Elbattah et al. (2017) explore learning about systems using machine learning toward more data-driven feedback loops. Their approach uses clustering to extract system structure from data, which then informs the construction of SD models. This work represents an early-stage exploration of data-driven SD model building, though practical applications remain limited and the methodology lacks robust validation frameworks.

The frontier of AI-assisted modeling is rapidly evolving beyond basic parameter estimation. Schoenberg (2026) explores the comprehensive role of AI in not only building but also learning with system dynamics models, suggesting a paradigm shift where AI actively assists in structural conceptualization and model formulation. Additionally, probabilistic structural approaches have been successfully integrated; Rodriguez-Ulloa (2018) combined Bayesian networks with systemic methodologies for risk evaluation, providing a probabilistic structure that complements the deterministic nature of traditional SD feedback loops.

Pushing structure discovery toward complete hybrid-model generation, Di Caprio & Leblebici (2026) propose SINDybrid, an algorithm that automatically constructs hybrid models of dynamic systems by combining sparse identification of nonlinear dynamics (SINDy) with optimization to decide which parts of a model should be represented mechanistically and which should be learned from data. Developed in a process-engineering context, the method illustrates how machine learning can be used not only to estimate parameters but to discover and assemble the structural form of a dynamic model, complementing the causal-loop-oriented structure-learning approaches discussed above.

4. Application Domains and Case Studies

The integration of System Dynamics and Machine Learning has been applied across diverse domains, each presenting unique challenges and opportunities for hybrid modeling approaches. The integration of SD and ML has proven versatile across a multitude of disciplines, addressing varying degrees of complexity and uncertainty. The distribution of case studies and applied research within the reviewed literature highlights distinct focal areas (Figure 8).

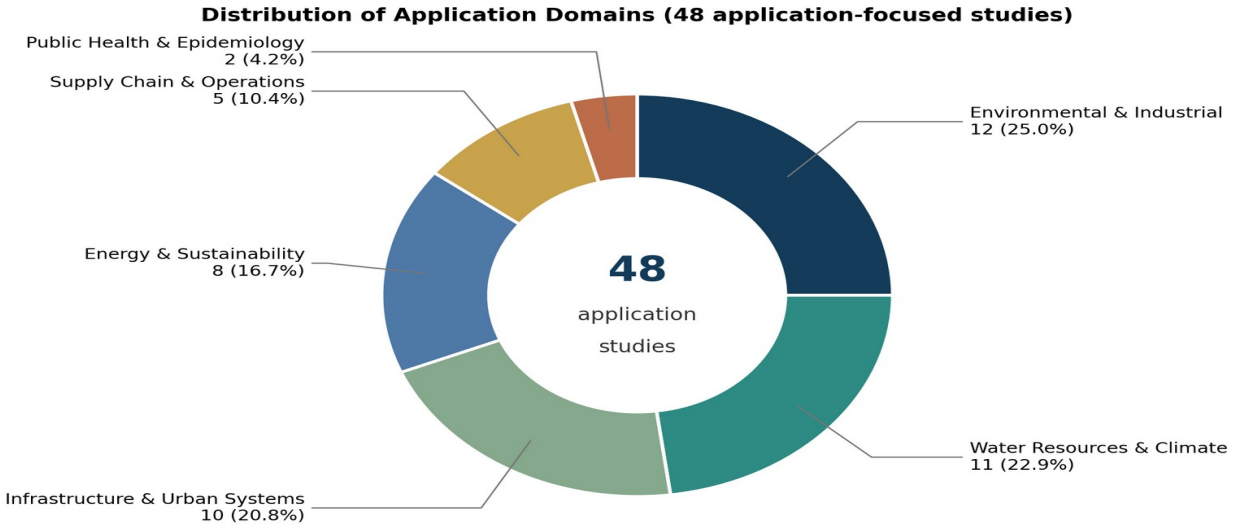

Figure 8. Distribution of application domains (48 application-focused studies).

Water resources and broad environmental systems collectively represent the largest share of applications. This concentration is largely driven by the urgent need to model long-term climate feedback loops (SD) alongside complex, high-dimensional climatic and ecological data sets (ML). The most recent 2026 studies reinforce this concentration, adding applications in climate-resilient viticulture, coastal eutrophication management, and land–water allocation, while also extending the field into sustainable transport and supply-chain risk detection.

4.1 Public Health and Epidemiology

Public health represents one of the most prominent application domains for SD-ML integration, driven by the need for both mechanistic understanding of disease transmission and data-driven parameter estimation. Gadewadikar et al. (2023) apply their AI-based parameter estimation methodology to a susceptible-infected-recovered (SIR) model using COVID-19 pandemic data, demonstrating how regression AI can continuously update model parameters as new epidemiological data becomes available. This application highlights the value of hybrid approaches during rapidly evolving public health crises where timely, data-informed predictions are critical.

Rahmandad et al. (2025) apply amortized Bayesian inference with deep learning to an epidemiological SEIRb model, achieving scalable parameter estimation for complex compartmental models. Their work demonstrates how advanced ML techniques can overcome computational bottlenecks in Bayesian calibration of epidemiological SD models, enabling more rigorous uncertainty quantification and faster response to emerging health threats. The public health domain benefits particularly from SD-ML integration because disease dynamics involve both well-understood mechanistic processes (suitable for SD) and complex, heterogeneous population behaviors (suitable for ML).

4.2 Water Resources Management and Climate Change

Water resources management, particularly under the stress of climate change, has emerged as a dominant application domain for SD-ML integration. Researchers frequently utilize SD to model the complex hydrological feedback loops and human consumption patterns, while employing data-driven models to handle uncertain climatic variables. Rahmati et al. (2022) and Zarghami et al. (2016) utilized SD approaches to manage multireservoir energy generation and reservoir operations under shifting climate impacts. Similarly, Babolhakami et al. (2023) applied these models to evaluate reservoir performance under future climatic scenarios.

Beyond reservoir management, hybrid models have been pivotal in regional water policies. Hosseini Baghanam et al. (2022) and Sheikhbabaei et al. (2022) leveraged SD approaches for integrated regional water resource management and policy-making under changing climate conditions. To address extreme weather impacts, Park et al. (2019) used modeling to evaluate water pricing policies for drought mitigation. Integrating cutting-edge remote sensing, Fernando et al. (2022) combined satellite laser altimetry (ICESat-2) with ML and SD models to estimate lake water levels and bathymetry, showcasing how advanced data collection methods can directly feed into dynamic simulation models. More recently, Jia & Zhang (2026) couple ML-generated climate scenarios with an SD model of soil moisture, yield, and basin-scale water allocation and use multi-objective optimization to derive Pareto-optimal irrigation and cropping policies for a rice–wheat system in the middle Yangtze River Basin under climate change.

4.3 Supply Chain and Operations Management

Supply chain management presents significant opportunities for SD-ML integration due to the combination of structural feedback effects (inventory dynamics, capacity constraints) and complex, data-rich operational patterns. Roozkhosh et al. (2022) develop a hybrid approach for predicting blockchain acceptance rates in resilient supply chains, using SD to model adoption dynamics and ML (MLP and SVR) for prediction. Their case study demonstrates how hybrid approaches can address both strategic (long-term adoption patterns) and operational (short-term acceptance rate prediction) challenges in supply chain innovation.

Sheikh et al. (2025) apply SD-ML integration to semiconductor manufacturing optimization for small and medium enterprises. Their hybrid framework addresses production planning, capacity management, and quality control, demonstrating practical value in manufacturing contexts. The semiconductor case study illustrates how SD can model production flows and capacity dynamics while ML handles demand forecasting and quality prediction based on complex process data.

Mamulak et al. (2024) integrate system dynamics with random forest algorithms for sales forecasting, showing how ML can enhance predictive accuracy in business planning while SD maintains the causal structure of market dynamics. This application demonstrates the value of hybrid approaches for tactical and strategic business decisions where both short-term accuracy and long-term structural understanding are required. Extending hybrid approaches to risk analytics, De-la-Cruz-Madrigal et al. (2026) integrate SD modeling with deep learning in an intelligent decision-support system that detects risk and disruption in supply chains, using SD to represent disruption-propagation dynamics and deep learning for predictive detection.

4.4 Energy Systems and Sustainability

Energy systems and sustainability applications leverage SD-ML integration to address multi-scale, multi-objective optimization challenges. Zhou et al. (2024) develop an intelligent framework for optimizing water-energy-food nexus synergies in urban metabolic landscapes, combining SD with ML for

sustainability analysis. This application demonstrates how hybrid approaches can handle the complex interdependencies and feedback loops characteristic of urban sustainability challenges while leveraging ML for pattern recognition in high-dimensional indicator spaces.

Rizqi et al. (2023) apply a hybrid system dynamics and adaptive particle swarm optimization (PSO) approach to green energy mix modeling under supply uncertainty. While PSO is not strictly machine learning, this work illustrates the broader trend of combining SD with computational intelligence techniques to address energy planning challenges. The energy domain benefits from SD-ML integration because energy systems involve both physical infrastructure dynamics (suitable for SD) and complex market behaviors and uncertainty (suitable for ML and optimization).

Kiluk (2017) uses diagnostic information system dynamics to evaluate machine learning algorithms for supervising energy efficiency in district heating-supplied buildings. This application demonstrates how SD can provide a framework for assessing and improving ML-based control systems, though the integration remains relatively loose with SD primarily serving as an evaluation tool rather than being tightly coupled with ML components.

The application of hybrid methodologies in energy systems continues to diversify. Ibrahim et al. (2023) advocate for a holistic approach to power systems using innovative ML and SD, addressing grid complexities. Focusing on the transition to renewable energy and smart mobility, Liu et al. (2018) utilized optimization techniques for electric vehicle charging station allocation by integrating charging satisfaction with distributed renewables, while Liu et al. (2019) modeled the dynamic evolution and sustainability of China's broader power supply and demand system.

4.5 Environmental and Industrial Systems

The integration of SD and ML is increasingly being applied to macroscopic environmental management, land use change, and ecosystem services. Highlighting the breadth of this domain, a recent comprehensive review by Nesanır et al. (2025) specifically focuses on the integration of SD and ML/AI in addressing general environmental matters. Building upon this context, specific applications demonstrate how hybrid approaches can address localized and global environmental challenges.

Environmental and industrial applications demonstrate the versatility of SD-ML integration across diverse system types. Shekhar et al. (2023) develop a hybrid mechanistic-machine learning approach to model industrial network dynamics for sustainable design of carbon capture and utilization technologies. This work exemplifies how hybrid approaches can combine mechanistic understanding of industrial processes with data-driven modeling of complex network interactions and market dynamics.

Arranz (2024) applies a system dynamics approach with machine learning to model eco-innovation drivers in companies, using SD to capture feedback mechanisms in innovation processes while employing ML to identify complex patterns in innovation adoption data. This application demonstrates the value of hybrid approaches for understanding organizational and technological change processes.

Crookes et al. (2016) use system dynamics for predator-prey analysis in the steel industry, comparing SD forecasts with neural network predictions. While this work treats SD and ML as separate tools rather than tightly integrating them, it illustrates the complementary insights that can be gained from applying both approaches to the same problem domain.

In specific applications, Huang et al. (2022) simulated future Land Use and Land Cover Change (LUCC) by coupling climate change and human effects using multi-phase remote sensing data. Expanding on ecosystem assessment, Zhang et al. (2024) explored future ecosystem service changes and their key

contributing factors, while Ouyang et al. (2022) focused on optimizing the spatial configuration of urban-agriculture-ecological functions in major urban agglomerations.

In the realm of waste and materials management, hybrid models offer significant predictive power. Vivekananda et al. (2014) combined multilinear regression with SD to forecast solid waste quantity and composition. More recently, Ajayi et al. (2025) integrated SD and ML to conduct environmental impact analyses of building materials during the demolition process, linking operational processes with long-term environmental outcomes. Participatory approaches have also been enhanced; Bertone et al. (2016) demonstrated how system approaches can improve environmental decision-making under high uncertainty by actively modeling with stakeholders.

In agricultural and ecosystem contexts, Borlinič Gačnik et al. (2026) integrate ML regressors with a stock-and-flow SD model to study climate-resilient viticulture, bridging ML-based prediction of wine quality with SD-based simulation of vineyard biomass dynamics and carrying-capacity constraints. In the marine domain, Lazăr et al. (2026) combine random forest, remote sensing, and SD to assess and mitigate eutrophication in the Romanian Black Sea coastal waters, using RF to identify nutrient drivers of chlorophyll-a and SD to simulate ecosystem responses under alternative management scenarios.

4.6 Infrastructure and Urban Systems

Infrastructure and urban systems represent emerging application areas for SD-ML integration. Sankaran et al. (2024) develop a system dynamics framework for human-machine learning decisions using New York Citi Bike as a case study. Their work explores how SD can model the feedback dynamics of bike-sharing systems while ML handles demand prediction and inventory optimization. This application illustrates the potential for hybrid approaches in smart city applications where operational ML systems interact with longer-term urban dynamics.

Zhang et al. (2017) use an integrated approach combining data mining and system dynamics for policy design, examining the effects of electric vehicle adoption on CO2 emissions in Singapore. This work demonstrates how data mining can inform SD model parameters and structure, enabling more data-driven policy analysis for urban sustainability challenges.

Infrastructure planning and smart operational control benefit substantially from AI-enhanced dynamic modeling. Demonstrating large-scale infrastructure applications, Rabelo et al. (2014) analyzed the expansion of the Panama Canal using simulation modeling combined with artificial intelligence. In transportation infrastructure, Ajorlou et al. (2024) applied data-driven sensitivity analysis to evaluate the performance of flooded flexible pavements under soil moisture fluctuations. Moving toward supply chain and logistics, Nitsche et al. (2022) employed SD modeling to design smart and collaborative last-mile delivery networks. Furthermore, hybrid models are proving effective in localized smart environments and public health applications; Chen et al. (2022) developed a smart microclimate control system for greenhouses using SD and ML techniques, and Qureshi et al. (2022) utilized neural network techniques for heat stress modeling, bridging environmental conditions with human health impacts. In sustainable transportation, Paul et al. (2026) couple an SD model of demand, travel distance, fuel price, and vehicle characteristics with ensemble machine learning and Sobol-based sensitivity analysis to predict the adaptability of vehicular transport systems under multiple future scenarios.

Extending hybrid modeling to safety-critical engineering, Udu & Okpala (2026) integrate machine learning, human factors, and system dynamics in a predictive framework for engineering safety in complex systems, using SD to capture the feedback structure of safety performance while ML predicts safety outcomes.

5. Current State-of-the-Art and Recent Advances

5.1 Advanced Inference and Uncertainty Quantification

The most significant recent advance in SD-ML integration is the development of sophisticated inference frameworks that combine deep learning with Bayesian methods. Rahmandad et al. (2025) represent the current state-of-the-art with their amortized Bayesian inference approach using neural posterior estimation. This methodology achieves several breakthroughs: (1) scalable likelihood-free inference for complex SD models, (2) instant generation of full parameter posteriors after neural network training, (3) rigorous uncertainty quantification, and (4) orders-of-magnitude computational speedup compared to traditional Bayesian methods. The approach addresses a fundamental limitation of SD modeling—the difficulty of rigorous parameter estimation and uncertainty quantification for complex models—while maintaining the causal structure and interpretability that make SD valuable for policy analysis.

This advance builds on earlier work in likelihood-free inference and simulation-based inference but represents the first comprehensive application to system dynamics models. The methodology opens new possibilities for real-time model calibration and adaptive policy-making, though it requires substantial upfront computational investment and expertise in both SD and deep learning.

5.2 Automated Structure Learning and Discovery

Recent advances in data-driven structure learning represent another frontier in SD-ML integration. Abdelbari et al. (2017) develop computational intelligence methods to learn causal loop diagram-like structures from observed data, addressing the traditional reliance on expert judgment in SD model building. While this approach remains in early stages, it points toward a future where SD models can be partially or fully constructed from data, potentially democratizing SD modeling and enabling discovery of unexpected feedback structures.

The challenge in this area lies in distinguishing genuine causal relationships from spurious correlations, a fundamental problem in causal inference. Current approaches lack robust validation frameworks and struggle with the complexity of real-world systems where multiple causal structures may be consistent with observed data. Nevertheless, this research direction holds significant promise for making SD modeling more data-driven and accessible.

More recent work extends this frontier from discovering causal-loop structure toward automatically assembling complete hybrid models, as in the SINDybrid framework (Di Caprio & Leblebici, 2026), which couples sparse identification of nonlinear dynamics with optimization to decide automatically which model components should be mechanistic and which should be learned from data.

5.3 Hybrid Mechanistic-Empirical Frameworks

The development of sophisticated hybrid frameworks that seamlessly combine mechanistic SD components with empirical ML components represents another important advance. Shekhar et al. (2023) exemplify this trend with their hybrid mechanistic-machine learning approach for industrial network dynamics. These frameworks recognize that real-world systems contain both well-understood mechanistic processes and complex phenomena that are best captured empirically. The key innovation lies in developing principled methods for determining which aspects of system behavior should be modeled mechanistically versus empirically, and how to ensure consistency and coherence across the hybrid model.

Recent work increasingly emphasizes the importance of maintaining interpretability and causal understanding even when incorporating ML components. This contrasts with earlier approaches that

sometimes treated ML as a “black box” add-on to SD models. State-of-the-art hybrid frameworks strive to preserve the explanatory power of SD while leveraging ML's pattern recognition capabilities.

5.4 Domain-Specific Integration Patterns

Recent literature reveals the emergence of domain-specific integration patterns tailored to particular application contexts. In public health, the pattern involves using SD for disease transmission dynamics and ML for parameter estimation from epidemiological data (Gadewadikar et al., 2023; Rahmandad et al., 2025). In supply chain management, SD models structural dynamics (inventory, capacity) while ML handles demand forecasting and operational optimization (Sheikh et al., 2025; Roozkhosh et al., 2022). In energy systems, SD captures infrastructure and policy dynamics while ML addresses uncertainty and optimization (Zhou et al., 2024; Rizqi et al., 2023). Recent 2026 studies reinforce these domain-specific patterns: in water and environmental management, SD captures hydrological and ecological feedback while ML supplies climate-scenario generation and driver identification (Jia & Zhang, 2026; Lazăr et al., 2026); in agriculture, ML predicts crop or product quality while SD simulates biomass and resource dynamics under carrying-capacity constraints (Borlinič Gačnik et al., 2026); in infrastructure, ensemble ML sharpens the predictive layer of SD sustainability models (Paul et al., 2026); and in supply-chain operations, SD represents disruption-propagation dynamics while deep learning provides predictive risk detection (De-la-Cruz-Madrigal et al., 2026); and in safety-critical engineering, SD represents the feedback structure of safety performance while ML predicts safety outcomes (Udu & Okpala, 2026).

These domain-specific patterns suggest that effective SD-ML integration requires careful consideration of domain characteristics and modeling objectives. The most successful applications demonstrate clear delineation of responsibilities between SD and ML components, with SD handling causal structure and long-term dynamics while ML addresses pattern recognition, prediction, and optimization in data-rich subdomains.

5.5 Research Clusters and Thematic Network

To understand the intellectual structure of the field, a keyword co-occurrence network was generated (Figure 9). As illustrated, the literature revolves centrally around 'machine learning', which acts as a primary hub branching out into specific methodological applications such as 'reinforcement learning', 'deep learning', and 'optimal control'. Furthermore, distinct clusters highlight the integration of these methodologies within structural domains such as 'power system dynamics' and 'nonlinear dynamical systems', underscoring the interdisciplinary nature of current research fronts.

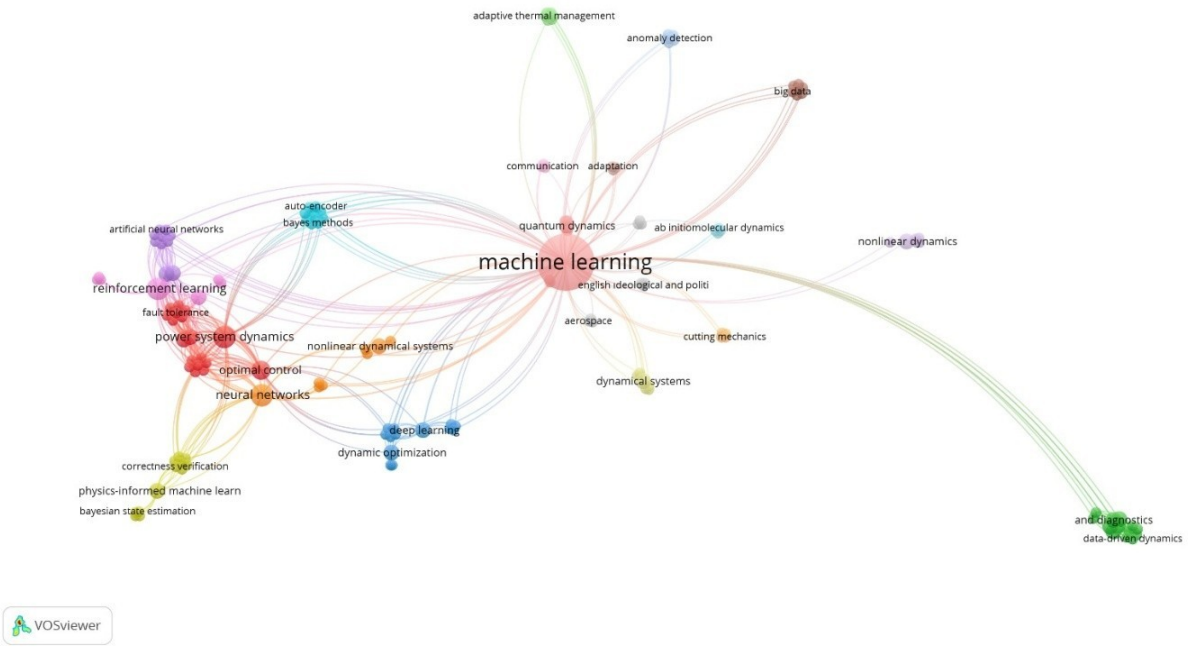

Figure 9. Keyword co-occurrence network map highlighting primary research themes and conceptual linkages. Source: vosviewer.org

5.6 Computational Tools and Platforms

Despite methodological advances, the development of standardized computational tools and platforms for SD-ML integration remains limited. Most studies implement custom integration solutions specific to their application domain and modeling objectives. Gadewadikar et al. (2023) describe an integrated environment for AI-based parameter estimation in SD models, but this remains a research prototype rather than a widely available tool. The lack of standardized platforms represents a significant barrier to broader adoption of SD-ML integration approaches.

Recent work increasingly emphasizes the need for open-source implementations and reproducible research practices. Rahmandad et al. (2025) provide code for their amortized Bayesian inference approach, facilitating replication and extension by other researchers. However, comprehensive platforms that support multiple integration patterns and provide user-friendly interfaces for practitioners remain absent from the literature.

6. Limitations and Challenges

Table 3 synthesizes the six principal limitation categories discussed in this section, mapping each to its core challenge, representative evidence from the reviewed literature, and a qualitative severity rating that reflects how strongly it currently constrains practical SD–ML integration.

Limitation Category	Core Challenge	Representative Evidence	Severity
Methodological foundations (§6.1)	No theory specifying when/why integration adds value; weak bidirectional coupling	Kamdem (2024); Abdelbari et al. (2017); Chen et al. (2011)	High
Scalability & computation	Heavy up-front training cost;	Rahmandad et al. (2025); Abdelbari	High

(§6.2)	combinatorial blow-up in structure learning	et al. (2017)	
Interpretability (§6.3)	ML “black boxes” erode the causal transparency that makes SD valuable	Schwaninger (2006); Elbattah et al. (2017); Edali (2022)	Medium
Data requirements & quality (§6.4)	ML data appetite dominates; errors propagate through feedback loops	Gadewadikar et al. (2023)	Medium
Generalization & transfer (§6.5)	Domain-specific solutions; transfer learning unexplored	Gadewadikar et al. (2023); Sheikh et al. (2025)	Medium
Software & tooling (§6.6)	No standardized platforms; custom code limits reproducibility	Gadewadikar et al. (2023); Rahmandad et al. (2025)	High

Table 3. Synthesis of key limitations of SD–ML integration.

Figure 10 visualizes these six limitation categories ranked by severity, complementing Table 3 by rendering its qualitative ratings in a directly comparable visual form. The chart separates the limitations into two tiers: those rated high severity—methodological foundations (§6.1), scalability and computation (§6.2), and software and tooling (§6.6)—which currently impose the strongest constraints on practical SD–ML integration, and those rated medium severity—interpretability (§6.3), data requirements and quality (§6.4), and generalization and transfer (§6.5)—which remain meaningful obstacles but are comparatively more tractable. Presenting the limitations in this ordered form clarifies where the field's most pressing challenges lie and motivates the prioritized research roadmap developed in the following section.

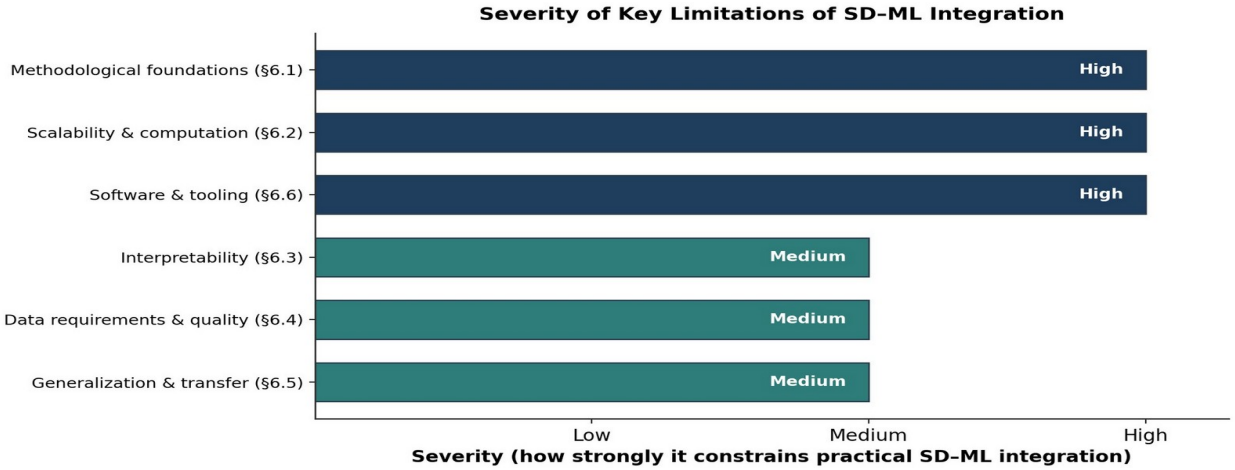

Figure 10. Severity of the six principal limitations of SD–ML integration (high severity in dark blue, medium in teal), as synthesized in Table 3.

6.1 Methodological Limitations

Despite significant advances, current SD-ML integration approaches face several fundamental methodological limitations. First, most integration methods lack rigorous theoretical foundations that specify when and why integration is beneficial compared to standalone SD or ML approaches (Kamdem, 2024). The literature provides numerous case studies demonstrating successful integration, but offers limited guidance on the conditions under which integration adds value versus adding complexity without commensurate benefits.

Second, validation methodologies for hybrid SD-ML models remain underdeveloped. Traditional SD validation emphasizes structural validity (correspondence between model structure and real-world causal mechanisms) and behavioral validity (correspondence between model behavior and observed system behavior) (Schwaninger, 2006). ML validation emphasizes predictive accuracy on held-out test data. Hybrid models require validation frameworks that address both causal validity and predictive accuracy, but such frameworks are largely absent from the literature (Abdelbari et al., 2017).

Third, most integration approaches treat SD and ML as separate components with limited bidirectional interaction. Gadewadikar et al. (2023) use ML to estimate SD parameters, but the SD model structure remains fixed. Roozkhosh et al. (2022) use SD to generate data for ML prediction, but the ML component does not feed back to refine the SD model. Truly integrated approaches where SD and ML components co-evolve and mutually inform each other remain rare (Chen et al., 2011).

6.2 Scalability and Computational Challenges

Scalability represents a significant practical limitation for many SD-ML integration approaches. Rahmandad et al. (2025) achieve scalable inference through amortized Bayesian methods, but this requires substantial upfront computational investment to train neural networks. For models that change frequently or applications where computational resources are limited, this approach may not be practical. Similarly, approaches that use ML for structure learning (Abdelbari et al., 2017) face combinatorial explosion as model complexity increases, limiting their applicability to relatively simple systems.

The computational challenges are particularly acute for real-time applications where rapid model updates are required. While some approaches promise “instant” parameter estimation after initial training (Rahmandad et al., 2025), the training phase itself may require hours or days of computation on specialized hardware. This limits the applicability of advanced SD-ML integration methods in contexts requiring rapid response to emerging situations.

6.3 Interpretability and Explainability

A fundamental tension in SD-ML integration concerns interpretability and explainability. System Dynamics models are valued for their transparency and ability to communicate causal mechanisms to stakeholders and policymakers (Schwaninger, 2006). Machine Learning models, particularly deep neural networks, are often criticized as “black boxes” that provide predictions without explanation (Elbattah et al., 2017). When ML components are integrated into SD models, there is a risk of compromising the interpretability that makes SD valuable for policy analysis.

Current approaches address this challenge with varying degrees of success. Some maintain clear separation between interpretable SD structure and ML components used only for specific tasks such as parameter estimation (Gadewadikar et al., 2023). Others attempt to extract interpretable insights from ML components (Edali, 2022). However, as integration becomes tighter and ML components take on more central roles in hybrid models, maintaining interpretability becomes increasingly challenging. The literature lacks systematic frameworks for preserving and communicating the causal insights of SD models when ML components are deeply integrated.

6.4 Data Requirements and Quality

SD-ML integration approaches often have substantial data requirements that may not be met in many practical applications. ML components require sufficient training data to learn accurate patterns, while SD models traditionally can be developed with limited data by leveraging expert knowledge and

theoretical understanding. When these paradigms are integrated, the data requirements of ML may dominate, potentially limiting applicability to data-rich domains.

Furthermore, data quality issues—missing values, measurement error, selection bias—can significantly impact ML performance and, by extension, the performance of hybrid SD-ML models. The literature provides limited guidance on how to handle data quality issues in hybrid modeling contexts, particularly when ML-estimated parameters are used in SD models where parameter errors can propagate through feedback loops and accumulation processes (Gadewadikar et al., 2023).

6.5 Generalization and Transfer Learning

Most SD-ML integration studies focus on specific application domains and case studies, with limited attention to generalization across contexts. A hybrid model developed for COVID-19 epidemiology (Gadewadikar et al., 2023) may not transfer easily to other infectious diseases or public health challenges. Similarly, approaches developed for semiconductor manufacturing (Sheikh et al., 2025) may not generalize to other manufacturing contexts. The literature lacks systematic investigation of which integration patterns and methodologies generalize across domains and which are inherently domain-specific.

Transfer learning—the ability to leverage knowledge gained in one context to improve performance in another—remains largely unexplored in SD-ML integration. While transfer learning is a major research area in machine learning, its application to hybrid SD-ML models is not addressed in the reviewed literature. This represents a significant missed opportunity, as SD models often encode generalizable causal knowledge that could potentially facilitate transfer learning across related domains.

6.6 Software and Tooling Gaps

The lack of standardized software tools and platforms represents a major practical barrier to widespread adoption of SD-ML integration approaches. Most studies implement custom solutions using combinations of SD software (Vensim, Stella, AnyLogic) and ML libraries (TensorFlow, PyTorch, scikit-learn), requiring expertise in both domains and significant software engineering effort (Gadewadikar et al., 2023; Rahmandad et al., 2025). User-friendly platforms that support common integration patterns and provide accessible interfaces for practitioners are largely absent.

This tooling gap has several consequences. First, it limits reproducibility, as custom implementations are often not shared or are difficult to replicate. Second, it raises barriers to entry for practitioners who may lack expertise in both SD and ML. Third, it slows the pace of methodological innovation, as researchers must repeatedly solve similar software integration challenges rather than building on standardized platforms. The development of open-source, well-documented platforms for SD-ML integration represents a critical need for the field.

7. Research Gaps and Future Directions

Table 4 organizes the ten gaps identified below into a prioritized research roadmap, rating each gap by urgency and positioning it on an indicative time horizon. Validation, uncertainty quantification, and standardized tooling emerge as the most pressing near-term priorities, whereas theoretical foundations and multi-paradigm integration are longer-horizon, higher-risk endeavours.

#	Research Gap	Future Direction	Priority	Time Horizon
7.1	Theoretical foundations for integration	Formal frameworks specifying when/why/how to integrate	High	Long-term

7.2	Validation & verification methodologies	Hybrid validity frameworks; shared benchmarks	Critical	Near-term
7.3	Bidirectional & co-evolutionary integration	Co-adaptive SD ↔ ML architectures; active learning	High	Mid-term
7.4	Scalability to large complex systems	Hierarchical, distributed, dimensionality-reducing methods	High	Mid-term
7.5	Causal discovery & structure learning	Causal algorithms tailored to stocks/flows/loops	High	Long-term
7.6	Domain-specific patterns & best practices	Cataloged patterns; reusable hybrid components	Medium	Near-term
7.7	Uncertainty quantification & propagation	Propagating ML uncertainty through SD feedback	Critical	Near-term
7.8	Standardized platforms & open-source tools	Common APIs; practitioner-friendly interfaces	High	Near-term
7.9	Ethical & societal implications	Bias, transparency, accountability frameworks	Medium	Mid-term
7.10	Integration with other paradigms	Three-way SD+ML+ABM; multi-paradigm frameworks	Medium	Long-term

Table 4. Prioritized research roadmap for SD–ML integration.

Figure 11 positions the ten research gaps of Table 4 on a priority-versus-time-horizon matrix, translating the roadmap into a visual representation intended to assist researchers and funding bodies in sequencing their efforts. The horizontal axis captures the time horizon over which meaningful progress can be expected, ranging from near-term to long-term, while the vertical axis reflects the relative priority of each gap, from medium to critical. Gaps that combine critical priority with a near-term horizon, such as uncertainty quantification and propagation (7.7), represent the most pressing opportunities and warrant immediate attention. By contrast, gaps located toward the long-term horizon, including causal discovery and structure learning (7.5) and integration with other modeling paradigms (7.10), are no less important but depend on foundational advances that must mature first. By making these trade-offs explicit, the matrix offers a practical guide for allocating research resources and establishing a coherent agenda for advancing SD–ML integration.

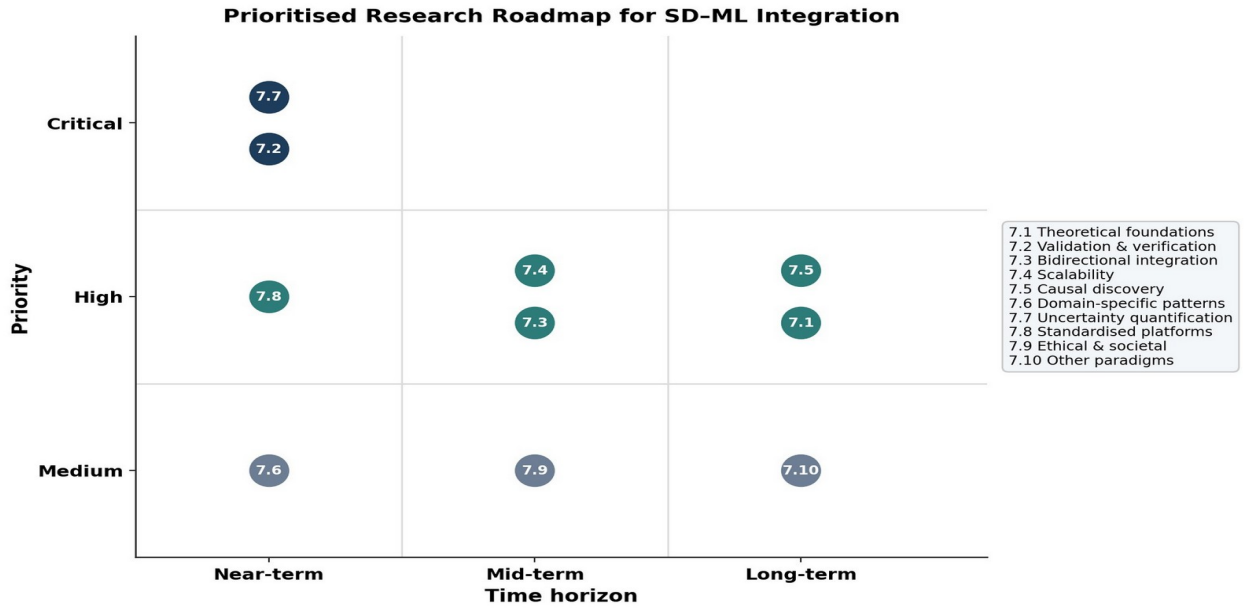

Figure 11. Prioritized research roadmap for SD–ML integration, mapping the ten gaps of Table 4 onto priority (medium–critical) and time horizon (near–long term).

7.1 Theoretical Foundations for Integration

Gap: The literature lacks comprehensive theoretical frameworks that specify when, why, and how SD and ML should be integrated. Current work is largely empirical and application-driven, demonstrating successful integration in specific contexts but providing limited theoretical guidance (Kamdem, 2024; Schwaninger, 2006).

Future Directions: Research is needed to develop formal theoretical frameworks that characterize the conditions under which SD-ML integration provides advantages over standalone approaches; specify principles for allocating modeling responsibilities between SD and ML components; establish theoretical guarantees for properties such as stability, convergence, and identifiability in hybrid models; and connect SD-ML integration to broader theories of hybrid modeling and multi-paradigm simulation. Such frameworks would provide principled guidance for researchers and practitioners, moving the field beyond ad-hoc integration approaches toward systematic methodologies grounded in theory.

7.2 Validation and Verification Methodologies

Gap: Rigorous validation methodologies for hybrid SD-ML models are largely absent from the literature. Traditional SD validation emphasizes structural and behavioral validity, while ML validation focuses on predictive accuracy, but integrated frameworks that address both dimensions are underdeveloped (Abdelbari et al., 2017).

Future Directions: Research should develop comprehensive validation frameworks that extend SD structural validity concepts to hybrid models with ML components; develop methods for validating the causal interpretations of ML-discovered structures; create benchmarks and test problems for comparing alternative integration approaches; establish standards for reporting validation results in hybrid modeling studies; and develop sensitivity analysis methods that account for both SD structure and ML component uncertainty. Robust validation methodologies are essential for building confidence in hybrid models and enabling their use in high-stakes policy and decision-making contexts.

7.3 Bidirectional and Co-evolutionary Integration

Gap: Most current integration approaches are unidirectional, with ML serving SD (parameter estimation) or SD serving ML (simulation environment), but lacking deep bidirectional interaction where components mutually inform and adapt to each other (Chen et al., 2011; Roozkhosh et al., 2022).

Future Directions: Research should explore co-evolutionary approaches where SD structure and ML components adapt simultaneously; feedback mechanisms where ML predictions inform SD structure refinement; active learning frameworks where SD models guide data collection to improve ML components; and meta-learning approaches that leverage SD causal knowledge to improve ML generalization. Bidirectional integration could unlock synergies beyond what current unidirectional approaches achieve, enabling hybrid models that are more adaptive, robust, and capable of continuous improvement.

7.4 Scalability to Large-Scale Complex Systems

Gap: Current SD-ML integration approaches have been demonstrated primarily on relatively small to medium-scale models. Scalability to large-scale systems with hundreds of variables, complex feedback structures, and high-dimensional state spaces remains largely unexplored (Rahmandad et al., 2025).

Future Directions: Research is needed on hierarchical and modular integration architectures that scale to large systems; distributed and parallel computation frameworks for hybrid SD-ML models; dimensionality reduction and model simplification techniques that preserve causal structure; efficient inference algorithms that scale to high-dimensional parameter spaces; and methods for managing computational complexity in real-time applications. Addressing scalability challenges is essential for applying SD-ML integration to grand challenges such as climate change, global health, and sustainable development that involve large-scale, complex systems.

7.5 Causal Discovery and Structure Learning

Gap: While Abdelbari et al. (2017) explore learning causal loop diagram-like structures from data, this research direction remains in early stages with limited validation and practical application. Robust methods for discovering SD model structure from data are largely absent.

Future Directions: Research should develop causal discovery algorithms specifically designed for SD model structures (stocks, flows, feedback loops); methods for combining expert knowledge with data-driven structure learning; validation frameworks for assessing the causal validity of discovered structures; approaches for handling confounding, selection bias, and other causal inference challenges in SD contexts; and interactive tools that support human-AI collaboration in SD model building. Advances in causal discovery could democratize SD modeling and enable discovery of unexpected feedback structures and causal mechanisms.

7.6 Domain-Specific Integration Patterns and Best Practices

Gap: While domain-specific applications are well-represented in the literature (Gadewadikar et al., 2023; Sheikh et al., 2025; Zhou et al., 2024; Roozkhosh et al., 2022), systematic characterization of domain-specific integration patterns and best practices is lacking. Each study tends to develop custom solutions without building on or comparing to related work in the same domain.

Future Directions: Research should systematically characterize integration patterns across application domains; develop domain-specific guidelines and best practices for SD-ML integration; create reference implementations and case studies for key application areas; investigate which integration approaches generalize across domains versus which are domain-specific; and build repositories of reusable hybrid

model components for common modeling tasks. Domain-specific knowledge synthesis would accelerate adoption and reduce the effort required to implement SD-ML integration in new applications.

7.7 Uncertainty Quantification and Propagation

Gap: While Rahmandad et al. (2025) make significant advances in uncertainty quantification for parameter estimation, comprehensive frameworks for uncertainty propagation through hybrid SD-ML models are lacking. How uncertainty in ML components propagates through SD feedback loops and accumulation processes is not well understood.

Future Directions: Research is needed on methods for propagating uncertainty from ML components through SD model structures; frameworks for quantifying and communicating total uncertainty in hybrid model predictions; sensitivity analysis methods that account for both parametric and structural uncertainty; approaches for decision-making under uncertainty with hybrid models; and validation of uncertainty quantification methods against real-world outcomes. Rigorous uncertainty quantification is essential for responsible use of hybrid models in policy and decision-making contexts where understanding the limits of model predictions is critical.

7.8 Standardized Platforms and Open-Source Tools

Gap: The lack of standardized, user-friendly platforms for SD-ML integration represents a major barrier to adoption. Most studies implement custom solutions that are not shared or are difficult to replicate (Gadewadikar et al., 2023; Rahmandad et al., 2025).

Future Directions: The field needs open-source platforms that support common SD-ML integration patterns; user-friendly interfaces accessible to practitioners without deep ML expertise; standardized APIs for connecting SD software with ML libraries; repositories of reusable hybrid model components and integration templates; comprehensive documentation, tutorials, and educational resources; and community-driven development and governance models. Standardized platforms would dramatically lower barriers to entry, improve reproducibility, and accelerate innovation in SD-ML integration methodologies.

7.9 Ethical and Societal Implications

Gap: The literature is largely silent on ethical and societal implications of SD-ML integration, including issues of algorithmic bias, transparency, accountability, and the potential for misuse of hybrid models in policy contexts.

Future Directions: Research should address how biases in training data propagate through hybrid SD-ML models; transparency and explainability requirements for hybrid models used in policy-making; accountability frameworks when hybrid models inform consequential decisions; potential for misuse or misinterpretation of hybrid model predictions; and ethical guidelines for developing and deploying SD-ML integration in sensitive domains. As hybrid SD-ML models are increasingly used to inform policy and decision-making, addressing ethical and societal implications becomes essential for responsible innovation.

7.10 Integration with Other Modeling Paradigms

Gap: The literature focuses primarily on SD-ML integration, with limited exploration of multi-paradigm integration involving agent-based modeling, discrete-event simulation, optimization, and other approaches (Schwaninger, 2006).

Future Directions: Research should explore three-way integration of SD, ML, and agent-based modeling; combining SD-ML with optimization and control theory; integration with discrete-event simulation for

operational contexts; multi-paradigm frameworks that flexibly combine SD, ML, and other approaches based on modeling objectives; and theoretical foundations for multi-paradigm integration. Expanding beyond two-paradigm integration could unlock additional synergies and enable modeling of systems that require multiple complementary perspectives.

8. Conclusion

The integration of System Dynamics and Machine Learning represents a promising and rapidly evolving research frontier that addresses fundamental limitations in both paradigms. This comprehensive literature review has synthesized findings from 58 studies spanning 2001–2026, revealing four primary integration approaches: ML-based parameter estimation, ML-driven policy optimization, hybrid simulation frameworks, and data-driven structure learning. Applications across public health, supply chain management, energy systems, manufacturing, and environmental sustainability demonstrate the broad applicability and practical value of SD-ML integration. The continued emergence of 2026 studies — spanning climate-resilient agriculture, coastal eutrophication management, land–water allocation, sustainable transport, supply-chain risk detection, engineering safety, and the automated generation of hybrid models, and originating from a widening set of countries including Slovenia, Romania, Mexico, Belgium, and Nigeria — confirms that the field is not only growing in volume but also diversifying in application scope and geographic reach.

Recent advances, particularly in amortized Bayesian inference for scalable parameter estimation (Rahmandad et al., 2025) and hybrid mechanistic-empirical frameworks (Shekhar et al., 2023), represent significant progress toward realizing the potential of integrated approaches. These advances enable more rigorous uncertainty quantification, faster model calibration, and seamless combination of mechanistic and empirical knowledge. Domain-specific integration patterns are emerging that provide guidance for practitioners in key application areas.

However, critical research gaps persist across multiple dimensions. Theoretical foundations for integration remain underdeveloped, with limited guidance on when and how to integrate SD and ML effectively. Validation methodologies for hybrid models lag behind methodological advances in integration techniques. Most current approaches involve unidirectional integration with limited bidirectional interaction between SD and ML components. Scalability to large-scale complex systems, robust causal discovery methods, comprehensive uncertainty quantification frameworks, and standardized computational platforms all represent significant gaps requiring future research attention.

The identified research gaps present substantial opportunities for advancing both theoretical understanding and practical implementation of hybrid SD-ML systems. Addressing these gaps will require interdisciplinary collaboration bringing together expertise in system dynamics, machine learning, causal inference, software engineering, and domain-specific knowledge. The development of rigorous theoretical frameworks, robust validation methodologies, scalable computational platforms, and domain-specific best practices will be essential for moving the field from ad-hoc integration approaches toward systematic, principled methodologies.

For researchers embarking on thesis work in this area, several high-impact directions emerge from this review. Developing comprehensive theoretical frameworks for SD-ML integration would provide foundational guidance for the field. Creating robust validation methodologies specifically designed for hybrid models would enable more rigorous evaluation and comparison of alternative approaches. Advancing bidirectional and co-evolutionary integration methods could unlock synergies beyond current unidirectional approaches. Building open-source platforms and tools would dramatically lower barriers

to adoption and accelerate innovation. Exploring causal discovery and structure learning could democratize SD modeling and enable data-driven discovery of feedback structures.

The integration of System Dynamics and Machine Learning holds significant promise for addressing complex societal challenges in public health, sustainability, infrastructure, and beyond. By combining SD's causal structure and policy analysis capabilities with ML's pattern recognition and predictive power, hybrid approaches can potentially overcome the limitations of each paradigm applied independently. Realizing this potential will require sustained research effort addressing the theoretical, methodological, computational, and practical challenges identified in this review. The field is poised for significant advances in the coming years, with opportunities for transformative contributions that bridge modeling paradigms and enable more effective analysis of complex systems.

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