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AI-EMPOWERED DATA-DRIVEN AGENT-BASED MODELING AND SIMULATION: CHALLENGES, METHODOLOGIES, AND FUTURE PERSPECTIVES

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ABSTRACT

Agent-based modeling and simulation (ABMS) has become one of the most popular simulation methods for scientific research and real-world applications. This tutorial paper explores recent development in the use of artificial intelligence including large-language models and machine learning, and digital twin in ABMS research. Given the different perspectives on ABMS, this paper will start with ABMS basic concepts and their implementation using an online platform called AgentBlock.net.

1 INTRODUCTION

The term *agent-based modeling* in this paper refers to the process of developing an *agent-based model* (ABM, the plural is ABMs). The running of an ABM which is typically done in the context of an experiment is referred to as *agent-based simulation* (ABS). The term agent-based modeling and simulation (ABMS) refers to the whole process of developing and using an ABM in a simulation study. ABMS has become a popular simulation method for scientific research and real-world applications (Macal 2016). The popularity of ABMS among the scientific community is demonstrated in the various simulation journals. Some journals in the field of Operations Research, Operations Management and Health Care also accept simulation as a valid method for research and decision support. In terms of applications, we can observe this from the many review papers on the applications of ABMS in various areas, such as business management (Onggo and Foramitti 2021), marketing (Negahban and Yilmaz 2014), food supply chain (Utomo et al. 2018), healthcare (Colasanti et al. 2022), and transportation (Huang et al. 2022).

This tutorial paper reviews the recent development in the use of artificial intelligence (AI), specifically large language models (LLMs) and machine learning (ML) as well as digital twin (DT) in ABMS research. Recently, there have been a significant development on AI and DT technologies. Hence, more and more ABMS research have incorporated these. Given the many different perspectives on ABMS, in section 2, we will first explain ABMS basic concepts and how they can be implemented using a tool called AgentBlock.net (He 2025a) that has a similar design to the Scratch programming language and provides a simple visual interface that helps beginners to learn ABMS more easily. Then, section 3 will focus on ABMS research that uses ML, LLMs and DT. Finally, section 4 concludes our paper with future research directions.

2 ABMS: CONCEPTS AND IMPLEMENTATION USING AGENTBLOCK.NET

This article use the following ABM definition: a simulation model that is formed by a set of autonomous agents that interact with their environment and other agents through a set of behaviors to achieve their objectives. In ABMS, modelers perceive the world as a set of interacting agents inhabiting in an environment. Hence, the main components of an ABM are agents, their behaviors and the environment where they live.

2.1 Agents

Agent definitions vary widely in complexity in the ABMS literature (Macal and North 2007). At one end of the spectrum, ABMs may consist of simple, homogeneous agents with basic behaviors. For example, in Schelling's segregation model (Schelling 1971), agents relocate until they reach a state of satisfaction. All agents behave identically and share the same threshold for happiness, making them homogeneous. At the other end, models may include heterogeneous agents exhibiting more complex behaviors such as perception, planning, and learning. A notable example is the social amplification of risk model (Busby et al. 2016), where agents—playing roles such as authorities, media, or members of the public—observe others' reactions to a risk event and adjust their own risk perceptions based on social feedback and cognitive biases. This contrast highlights the range of agent complexity in ABMS.

This article uses the following definition for agent: an entity that can make an independent decision in order to achieve its objectives. An agent can be human or non-human (e.g. an organization, a drone) as long it can make a decision or the behavior is important. An agent has a set of properties (or attributes) that characterized the agent. The properties can be in the form of a simple value such as happiness threshold in Schelling (1971), or a complex concept such as memory and belief in Busby et al. (2016).

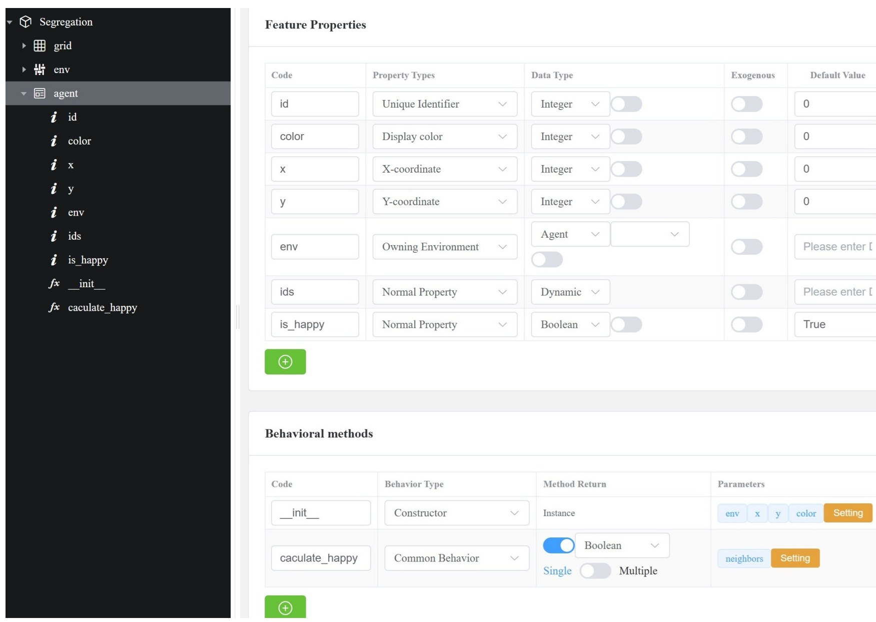

Figure 1: Defining agent properties and behaviors in AgentBlock.net.

2.2 Agents Behaviors

Agents are autonomous, i.e. they can make independent decisions (or behaviors) which can be *immediately observable* by other agents such as physical movements, purchasing a product or service, posting a review, sharing information and consuming shared resources from the environment, or *unobservable* behavior that changes the internal attributes of an agent such as belief and satisfaction level. These behaviors are not directly observable by other agents but they may affect the observable behaviors. Figure 1 shows how to define agent's properties and behaviors in AgentBlock.net.

An important behavior that justifies the use of ABMS is the interaction between agents. It is the interaction between agents that can generate the non-linearity and emergence behavior. The interactions between agents can produce non-linearity where a small change in individual agent's behavior lead to a disproportionate change at the system level. Emergence behavior is a certain pattern that appears at the population level as a result of the interactions between agents. Examples include the formation of ghettos in Schelling's segregation model and the public amplification of risk in the social amplification of risk model. Both emergent behaviors are not explicitly programmed into the model; instead, they arise from the independent decisions made by agents, for example, relocating when agents are unhappy in the segregation model or adjusting risk perception in the social amplification of risk model. A key advantage of ABMS lies in its ability to generate and explain emergent behavior resulting from local interactions among agents. These behavioral rules are followed because each agent acts to achieve its own objectives, such as seeking happiness in the segregation model or minimizing risk exposure in the social amplification of risk model.

2.3 Environment

In an ABM, the environment can be either spatial or relational. A spatial environment represents the physical location where an agent exists (e.g. city). Commonly used spatial environment types in ABM include grid, continuous space (or Euclidean space), and Geographical Information System (GIS). A grid divides space into structured cells across one or more dimensions. This structure is commonly used in many ABMs including the segregation model. In contrast, an n-dimensional continuous space represents an agent's location as a vector $(x_1, x_2, \ldots, x_n)$, providing a more realistic spatial environment than a grid. The most lifelike spatial representation is achieved using GIS, which model agents within real-world geographical areas. In contrast, a relational environment defines the connections between agents whether physical, such as transportation network, or non-physical such as those found in social networks. Networks in a relational environment can be constructed either empirically using real-world network data or theoretically through algorithms such as small-world, scale-free, or random network models.

The environment plays a crucial role in an ABM, as it can influence agents and their behaviors. For instance, in the segregation model, an agent decides whether to move or stay based on the composition of its neighborhood. Similarly, in the social amplification of risk model, an agent adjusts its risk perception by observing the actions of others. Additionally, the environment can serve as a medium for indirect interactions between agents. In such cases, an agent may alter the environment, which in turn impacts other agents. For example, in the segregation model, when an agent relocates, it changes the conditions of both its previous and new neighborhoods, influencing the decisions of other agents in those areas.

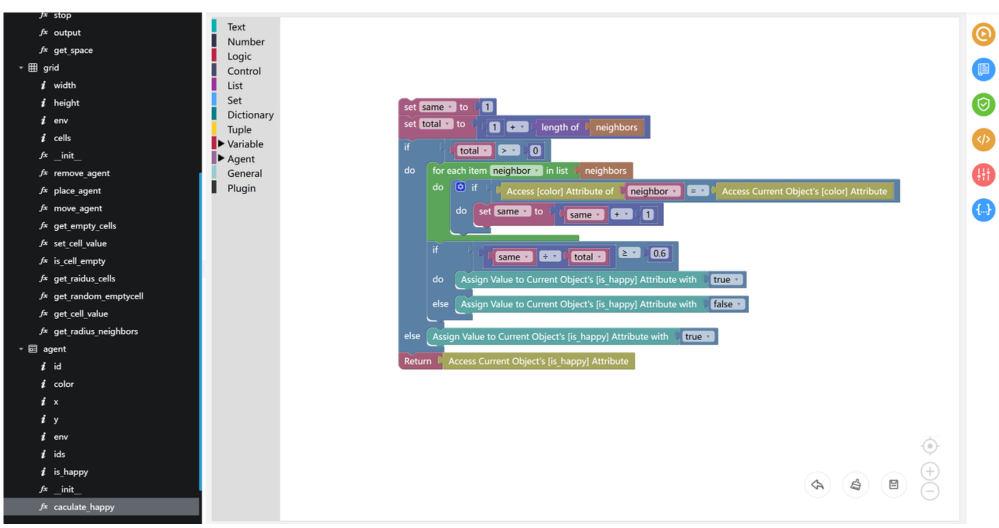

Figure 2: The Blocks of the Schelling Model.

2.4 Implementation using AgentBlock.net

ABMS is an important tool for analyzing complex systems, but its adoption in academia faces several hurdles. These include the need for programming expertise, difficulty in replicating existing models, and a lack of unified platforms for model reuse. AgentBlock.net aims to overcome these limitations. It offers a structured, user-friendly environment that combines visual programming, reusable modular components, and end-to-end workflow support. The visual interface, built on Google Blockly, lets users construct models using drag-and-drop operations (Figure 2). The code is available from He (2025b). This method abstracts complex coding, allowing users to build models with pre-defined blocks that encapsulate core ABM components, removing the need for traditional programming knowledge. AgentBlock.net offers several advantages for ABMS research:

- **Simplifies Model Development**: AgentBlock.net reduces the technical barriers associated with traditional ABM. It removes the need for extensive programming skills, allowing researchers to focus on theoretical aspects rather than technical implementation. This streamlines the process of translating concepts into executable simulations.
- **Boosts Reproducibility and Reusability**: The platform addresses issues with replicating and extending ABMs by providing a standardized, modular library. This library contains reusable core modules for agents, behaviors, and environments. Users can leverage pre-validated modules or contribute their own, with built-in version control and documentation to support transparency and reuse.
- **Facilitates Seamless Collaboration**: The platform offers a unified workflow for model design, simulation, and sharing. Users can build models visually, run them in-browser with live visualizations, and share permanent links that include all necessary code and settings. This approach streamlines collaboration, enabling easy exploration, validation, and extension of models by others.
- **Promotes Cross-Disciplinary Innovation**: AgentBlock.net supports multidisciplinary compatibility, allowing researchers from various fields (e.g., management science, sociology, economics) to integrate diverse theories and methods. Its standardized module interfaces enable combining different models, such as combining consumer behavior models from economics with social network structures, or environmental simulations with optimization techniques; hence, fostering hybrid approaches and cross-disciplinary collaboration for analyzing complex real-world systems.
- **Enhances Scholarly Rigor**: The platform allows researchers to link published work directly to corresponding computational models and modules. This bridges a common gap in ABMS research where theoretical contributions are often disconnected from their technical implementations, thereby improving scholarly rigor.

3 AI-EMPOWERED DATA-DRIVEN ABMS

As the field has matured and the volume of available data continues to grow, there is increasing emphasis on grounding agent-based models in empirical evidence. Such data are used to enhance model realism by informing agent characteristics, behaviors, and interactions; generating representative agent populations; and constructing realistic environments. Empirical data also enables more rigorous model validation by comparing simulation outputs with observed data. This section discusses how we leverage the increasing amount of data by integrating ABMS with Machine Learning, Large Language Models and Digital Twins.

3.1 ABMS and Machine Learning

Machine Learning (ML) is a multidisciplinary field that improves task performance through data-driven analysis and processing (Mitchell et al. 1986). Unlike traditional programming, ML algorithms learn autonomously from data using statistical techniques to identify patterns and make predictions (Dehkordi et al. 2023). This makes ML a strong complement to conventional statistical modeling (Valletta et al.

2017). A key advantage of ML is its ability to uncover patterns directly from raw data without predefined relationships, supporting flexible and scalable data analysis (Sivakumar et al. 2022). The increasing volume of data makes ML's role in ABMS research increasingly important. The fundamental steps when using big data and ML in ABMS can be delineated as follows:

1. **Data Acquisition and Preprocessing)**: This initial stage involves collecting large and diverse datasets (e.g., social media feeds, mobile phone traces, survey responses) (Kavak et al. 2018), and performing thorough cleaning, transformation, and feature engineering to prepare them for modeling (Sassite et al. 2022).
2. **ML-Driven Behavior Induction**: ML techniques extract behavioral rules and agent attributes from the preprocessed data. This can involve supervised learning for predicting decisions or unsupervised learning to uncover hidden patterns. For instance, decision trees, association rule mining, or neural networks can infer agent reactions or categorize behaviors (Turgut and Bozdag 2023) with feature importance ranking informing agent decision-making.
3. **ABM Construction and Simulation**: Insights from ML are integrated into the ABM. Agents are endowed with ML-derived behaviors and attributes, and their interactions are simulated. This allows researchers to observe emergent phenomena and system-level dynamics.
4. **Model Validation and Iteration**: Simulation outputs are rigorously compared against empirical data to ensure validity (Kavak et al. 2018). This may involve comparing simulated aggregate patterns with real-world observations or employing statistical methods to assess the model's accuracy. Discrepancies necessitate iterative model refinement, potentially adjusting ML-derived behaviors or ABM interaction rules.
5. **Analysis and Interpretation**: This final step involves analyzing simulation results to gain insights. This includes exploring system sensitivity, identifying key drivers of emergent phenomena, and evaluating potential interventions.

This integrated approach combines the strengths of ML and ABM, enabling more empirically grounded and nuanced explorations of complex social systems. While simulating complex systems presents challenges in handling massive datasets, improving accuracy, and optimizing efficiency, the combined ML and ABM paradigm offers a way to address these issues. Current research in this area are as follows.

3.1.1 Improving the Accuracy of Agent Behavior Model

In ABMS, accurately modeling individual agent behavior is critical. Agent behaviors are typically elicited using methods such as survey, interviews, focus group discussions, participatory modeling, or games. The availability of big data enables ML methods (e.g. reinforcement learning and supervised learning) to infer agent behaviors more precisely by leveraging extensive real-time and historical data for improved behavior modeling (Kavak et al. 2018). Van Dam et al. (2012) suggested that improving the accuracy of agent behavior modeling directly influences the predictive power of system behavior. Consequently, leveraging big data and ML not only strengthens the effectiveness of ABM but also potentially boosts prediction accuracy, ensuring that the model better captures the complexities of dynamic behaviors.

An example of how the elicitation of agents' decision rules from big data using ML can help improve the performance of ABM is shown in Turgut and Bozdag (2023). In their study simulating population mobility of Burkina Faso, ML is used to predict residents' migration decisions from survey data, comprising 3,500 households and over 8,000 respondents, with personal information including marital status, age, gender, and education level Turgut and Bozdag (2023). Then three tree-based models (decision tree, random forest, and XGBoost) were applied to predict residents' migration decisions (1 for migration, 0 for non-migration) from the survey data. Finally, XGBoost prediction results (the best performing model in this experiment) were used to guide agent decision making, and ABM simulations were performed to replicate the overall migration patterns of 4,449 simulated individuals observed between 1970 and 1999. The results demonstrate that the ML-driven ABM simulation (MAPE=8.81%) achieved superior performance compared to conventional ABM simulations (MAPE=10.11%).

Black box model and explainability: Although ML significantly enhances model prediction accuracy, it's a black box that makes it difficult to understand how decisions are made (Rudin 2019). By incorporating explainable ML techniques, such as LIME and SHAP, the transparency of the inferred behavior can be greatly improved, enabling researchers to gain deeper insights into the decision-making processes behind these models (Pillai 2024). On the other hand, when the decision rules in an ABM is too complex, integrating ML into ABMS can also improve the interpretability by treating a subset of the decision model as a blackbox and making the decision rules simpler.

3.1.2 Inferring Agent Behaviors

Big data delivers a rich, multi-dimensional, and vast volume of information. ML techniques can identify valuable patterns and trends within this data that can potentially be missed when eliciting agent behaviors using methods such as interviews or focus group discussions. The following two examples demonstrate the use of ML to infer agent behaviors.

Pouladi et al. (2020) constructed a social hydrological mixed model consisting of ML and ABM by combining agricultural, hydrological, and questionnaire survey data to study how farmer activities affect the local hydrological environment. The apriori association rule algorithm was used to extract 9 crop selection rules with high confidence values from the questionnaire survey data to guide farmers' activities in ABM. For example, if farmers have poor economic conditions, their farms are located next to crack diversion dams, have a water well, and can use the main irrigation canal, they tend to choose to plant alfalfa, and the confidence level of this rule is 82%. The results of ABM indicate that economically disadvantaged farmers will maximize profits by planting water consuming crops such as alfalfa and sugar beets, and meet irrigation needs through illegal groundwater wells, which have led to the shrinkage of Lake Urmia.

Augustijn et al. (2020) used ML to predict residents' perception of cholera risk while simulating the cholera outbreak in Kumasi, Ghana. A questionnaire survey was conducted on participants from 92 countries in MOOC to obtain their willingness to use water sources with different pollution levels under different conditions. Then, decision tree C4.5 was used to rank the importance of factors that affect cholera risk perception. The results indicate that in the perception of cholera risk, media is the most important followed by memory, visual pollution, and neighbors. The study shows that sensing the risk of cholera outbreaks faster can effectively reduce cholera cases.

Noise and data uncertainty: Data is often characterized by noise and uncertainty, and handling big data typically requires robust preprocessing capabilities, with ML playing a pivotal role in this process (Hariri et al. 2019). Through techniques such as data cleaning, feature extraction, and pattern recognition on large-scale, multi-dimensional datasets, ML can effectively extract meaningful insights and provide precise input for ABMS (Dehkordi et al. 2023). For instance, data mining methods can uncover latent patterns in agent behavior from historical data, further enhancing the behavior modeling process (Sivakumar et al. 2022). Gudivada et al. (2017) highlight that data quality issues are a primary factor hindering the progress of ABMS, underscoring the critical importance of big data preprocessing and ML in effective data modeling.

3.1.3 Improving Computational Efficiency

ML has been used in developing a surrogate for computationally expensive ABM. The surrogate model (e.g. artificial neural network, regression model) can quickly estimate the input-output transformation done by the ABM. Hence, it can be used to replace the ABM in a large scale simulation optimization or sensitivity analysis experiments. Pietzsch et al. (2020) provide a review on this topic.

3.2 Generative AI and Large Language Models in ABMS

Generative AI (GenAI) and large language models (LLM) are driving the fourth AI boom, with applications spanning a wide range of domains (Tu et al. 2024). Unlike previous waves, which focused on narrow, task-specific AI systems, such as rule-based approaches, statistical learning, and deep learning, LLM and GenAI are underpinned by foundation models with generative capabilities. These models can understand, generate, and manipulate human-like text, images, audio, and code. Exemplified by systems such as GPT (OpenAI 2023), Claude (Anthropic 2023), and DALL·E (Ramesh et al. 2022), they demonstrate remarkable versatility, supporting use cases ranging from creative content generation to human-like reasoning and problem solving.

In the context of ABMS, traditional ABMS systems rely heavily on predefined rules or probability-based behaviors encoded in agents to simulate complex systems. However, these models often suffer from rigid semantics and limited adaptability, especially when modeling human behaviors and social systems. By integrating GenAI and LLMs, ABMS systems can gain a deeper understanding of context, intent, and nuanced interactions. LLMs can be used to generate or refine agent behavior rules based on natural language descriptions, enabling domain experts to define and modify agent logic more intuitively. This semantic enrichment bridges the gap between high-level conceptual modeling and low-level implementation, making ABM more accessible and accurate. Moreover, LLMs can help agents reason, explain decisions, and interact in more human-like ways. For example, agents powered by LLMs can engage in natural dialogue, understand evolving social dynamics, or even simulate cognitive processes such as planning, negotiation, and emotion. Additionally, GenAI tools can assist in translating qualitative data (e.g., interview transcripts, field notes) into structured agent rules, enabling the construction of models that are grounded in real-world observations while maintaining semantic richness.

3.2.1 GenAI and LLM Tools

Most GenAI tools are built on top of transformer-based LLMs such as OpenAI's GPT series, Google's Gemini, Meta's LLaMA, Anthropic's Claude and Tesla and xAI (Grok). These models are pre-trained on vast corpora and then fine-tuned or aligned using techniques like instruction tuning and reinforcement learning with human feedback to serve as interactive, secure and task-specific tools.

Generative Pre-trained Transformers (GPTs) are the foundational models behind the ChatGPT family (OpenAI 2023). Owing to their ability to generate human-like text, GPT models have been increasingly applied in ABMS across various domains. For example, GPT models have been used in social simulation to empower the agents' interactive behaviors at a language level (Gürcan 2024). Hu et al. (2024) utilized the "GPT-3.5-turbo" model to simulate user-generated posts during information propagation processes. With the emergence of LLM bots on social media, LLM-BotGuard (Duan et al. 2025) was developed as an LLM detection framework designed to identify GPT-like, LLM-driven social media bots based on their unique characteristics. Empowered by the "GPT-3.5-turbo-16k" version of ChatGPT, LLM-based agents have demonstrated coordinated behavior, exhibiting human-like reasoning and task-specific competencies in a specialized job recruitment scenario (Li et al. 2023).

DeepSeek (Liu et al. 2024) is a series of open-source language models. It emphasizes enhanced multilingual reasoning capabilities, making it well-suited for cross-domain simulation tasks that require complex inference and decision-making. They are known as cost-effective because of their innovated Mixture-of-Experts (MoE) structure and effective training and software implementation. Wang et al. (2025) applied DeepSeek-v2 (Liu et al. 2024) to simulate a dynamic financial market, where the LLM agent is built upon a hierarchical knowledge architecture that integrates domain-specific financial expertise while also exhibiting behaviorally consistent forms of irrationality.

Another open-source AI models, Llama series (Touvron et al. 2023), developed by Meta, provide accessible yet powerful LLMs tailored for efficient deployment and fine-tuning, thereby significantly lowering computational barriers and facilitating broader adoption in ABMS scenarios, particularly in environments with constrained computational resources. In addition to their demonstrated interactive and collaborative behaviors, LLM agents also exhibit the ability to self-evolve, as shown in AlpacaFarm (Dubois et al. 2023). In this work, the "LLaMA 7B" model was fine-tuned to simulate human feedback, thereby helping to reduce training costs.

However, challenges remain regarding computational cost, integration complexity, and the need for specialized expertise to fully leverage LLMs within the ABMS framework. Moreover, research on LLM-based ABMS is still limited (Siebers 2025). LLM-AIDSim (Zhang et al. 2025) represents one of the earliest explorations of applying LLMs in ABMS.

3.2.2 LLM-AIDSim: A LLM-Empowered ABMS Tool

LLM-AIDSim (Zhang et al. 2025) is a LLM-enhanced ABS tool designed to model information propagation on social networks. In particular, LLMs are used to model social network users, enabling language-level inference and understanding of user agents. As a result, public opinions can be summarized after multiple rounds of simulation, supporting policy makers in shaping the desired spread of public statements.

In the context of public communication, the content of a statement is critical for organizations, governments, or businesses to effectively spread their ideas, policies, or new products. However, this diffusion is somehow unpredictable. Simulating potential public concerns before its release can help address this challenge. Although influence diffusion models are widely applied to simulate information propagation, these models face some challenges. In traditional influence diffusion models, individuals' decision-making behaviors are based on a certain probability. Though ABM has been incorporated into these models to emphasize the distinctive personalities and the complex interactive behaviors of individuals (Li et al. 2023), most of ABM approaches overlook the language-level abilities of user agents. Also, the alteration behavior of user agents are often ignored in these models (Wang et al. 2023). **LLM**-enhanced **A**gent-based **I**nfluence **D**iffusion **Sim**ulation (LLM-AIDSim) is a novel simulation tool built upon an LLM-empowered influence diffusion model developed for social networks. It addresses existing gaps by leveraging LLMs for generating user agent profiles, as well as generating and updating user agents' responses. Figure 3 illustrates the framework of LLM-AIDSim.

LLM-AIDSim executes simulations based on real-world social network topologies to better reflect realistic dynamics. Simulation parameters and diffusion model configurations are set by end-users through a web-based interface. To generate representative user profiles, the large language model "llama3:8b" is used to generate user profiles. Moreover, demographic data collected from public census sources, including distributions of age, gender, salary, education level, and occupation, are incorporated into the generation prompts, making the resulting user profiles more representative of real-world populations.

In the simulation stage, the LLM model is employed as the "brain" of each user agent to generate a response to the initial spreading message based on its profile. Additionally, with a certain probability, a user agent may revise its response after observing the reactions of its neighbors. This dynamic updating process is also powered by the LLM.

After several rounds of simulation, LLM-AIDSim collects the posts generated by user agents and conducts a detailed semantic analysis, which includes: (1) comparison with real-world comments; (2) topic evolution and convergence tracking; (3) clustered topic analysis; and (4) evaluation across different LLM models. The comparison with real-world comments and the evaluation of different LLM models are used to validate the simulation's reliability and adaptability. Topic analysis reveals potential public concerns, thereby supporting informed decision-making in the crafting of public statements.

3.3 ABMS and Digital Twins

The Digital Twin (DT) concept, introduced by Grieves and Vickers in 2003, involves a physical object, a virtual replica, and their connection (Grieves and Vickers 2017). Kalyani and Collier (2024) further refined this, defining DT as "the creation of a virtual/digital replica or model of a physical entity—such as a machine, building, farm, or person—using real-time data collected from the physical object to construct

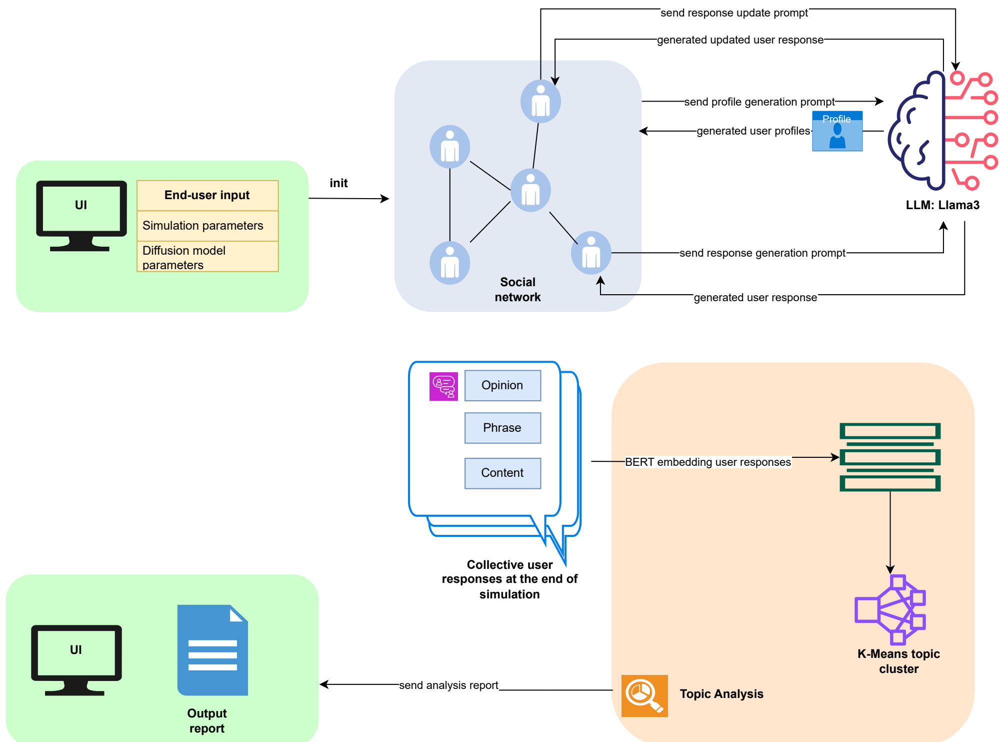

Figure 3: LLM-AIDSim Framework (Zhang et al. 2025).

the digital counterpart or model." DTs can leverage ABMS to better model dynamic agent behaviors and their emergent behaviors (Abdelalim et al. 2024). While DTs offer real-time data and system architecture, ABMS allows for simulating individual-level decisions and interactions, revealing system-level dynamics. This integration is especially useful (but not exclusively) for social systems.

Unlike engineering systems, social systems consist of diverse, autonomous, and adaptive agents influenced by preferences, norms, and constraints, leading to high complexity and uncertainty (Lansing 2003). ABMS is well-suited for simulating social systems due to its ability to model from the bottom-up, represent individual differences, and capture emergent behaviors (Helbing 2012). This makes ABMS crucial for building DTs for social systems, accurately reflecting their complexity and heterogeneity. Furthermore, ABMS's adaptive nature allows agents to adjust behaviors and goals dynamically within the DT in response to changing conditions (Kalyani and Collier 2024). This capability is especially important for modeling real-world scenarios such as policy interventions, emergency responses, or environmental changes. This integration enables social DTs to accurately represent social mechanisms and serve as platforms for counterfactual experiments and decision support. (De Marchi and Page 2014). By incorporating real-time data, DTs provide ABMs with dynamic input (Liu et al. 2024), improving their responsiveness and adaptability. This data-driven support helps validate agent behavior, enhancing the realism and credibility of ABMS and strengthening the capacity for high-fidelity social system modeling and forecasting.

3.3.1 Mechanisms of ABM-DT Integration: From Individuals to Cities

The fundamental principle behind the integrated ABM-DT lies in the close coupling of physical systems with virtual models through real-time data, forming a dynamic feedback loop. DT collect data from the physical world in real-time using sensors and IoT devices and map this data onto virtual models, while ABM simulates individual behaviors and interactions of agents within a system (Tzachor et al. 2022). By integrating ABM's behavioral simulations with the real-time data from DT, the system's behavior can be dynamically adjusted and optimized, future states can be predicted, and decision support can be provided under various strategies (Marçal Russo et al. 2025).

The construction of DT for social systems requires hierarchical mapping from macro to micro scales. It begins with the integration of static data such as roads, buildings, population, and infrastructure at the city level, combined with GIS and IoT for dynamic updates, forming the digital backbone of the urban lifeline. Building on this, community-level data such as room layouts, population movement, and service facilities are refined, with real-time calibration of local states through sensors and monitoring networks. Ultimately, the modeling of individual agents is implemented, defining attributes and behavioral rules for entities such as residents and businesses, using mobile trajectories and social data to drive micro interactions (Hii and Hasama 2024). To connect different layers, ABMS is used for bottom-up simulation of individual interactions leading to emergent macro phenomena, while DT inject city dynamics into the agent environment top-down. The key to their integration lies in designing multi-scale interaction rules, allowing agents to respond to policy changes, environmental events, and other global influences, continuously calibrating the model through multi-source data such as satellite remote sensing and social networks (Shtaierman et al. 2025). This approach retains ABM's explanatory power for complex social behaviors, while also incorporating the real-time capabilities of DT, ultimately forming a multi-layered, closed-loop feedback virtual social system from individuals to cities, providing a dynamic simulation platform for urban planning, crowd control, emergency or disaster management, and more.

3.3.2 Examples of ABM-DT Integration in Social Systems

Digital Twins (DTs) are crucial for various social system applications. In urban traffic management, DTs simulate real-time traffic, vehicle behavior, and road conditions to provide accurate decision support. This optimizes resource allocation, reduces congestion, and improves road safety (Bao et al. 2021). For the circular economy, DTs enhance transparency, resource flow, and management efficiency by providing real-time data across the entire product lifecycle. This optimizes data flow from design to recycling, improving resource use, reducing waste, and fostering stakeholder collaboration for more sustainable resource management (Preut et al. 2021). DTs also play a key role in disaster emergency management. By integrating diverse data, AI, and game theory, they offer accurate situational assessments, optimize resources, and facilitate multi-party coordination. During a disaster, DTs gather real-time data from sources like satellites, drones, and social media to analyze dynamic changes, supporting emergency managers' decisions (Fan et al. 2021). This approach can also be adapted to simulate COVID-19 transmission in urban areas by integrating individual agents, viral variants, vaccination parameters, and intervention measures to evaluate their collective impact on epidemiological outcomes (Barat et al. 2022).

There are several reported cases that combine DT with ABM. For example, Singapore has created the world's largest digital twin city. It utilizes DT integrated with ABM to optimize traffic and enhance urban mobility (Faliagka et al. 2024). The Port of Rotterdam in the Netherlands has developed a DT to monitor port operations in real time (Klar et al. 2023). Shenzhen has constructed a city-scale DT by integrating multi-source spatio-temporal data, enabling real-time visualization, computation, and simulation across various domains such as infrastructure, transportation, population, and the environment (Li et al. 2025).

3.3.3 The Case of Wuhan Large-Scale Social Simulator

This section presents a case from China: the Wuhan Large-Scale Social Simulator, developed by PKU-Wuhan Institute for Artificial Intelligence, which exemplifies the integration of DT and ABM approaches in the context of urban social systems. By building a city level virtual simulation platform that can respond in real-time, it is used to simulate residents' behavior, assist in urban governance and decision support.

As Figure 4 shows, the Large Social Simulator (LSS) integrate the approaches of DT and ABM. Big data such as detailed road and building information are used to construct the environment so that the simulator can reflect and visualize the real Wuhan city. As the real data streams like traffic information, power usage, internet bandwidth usage plugged in, we can construct the DT of the city and each community inside it. However, gathering individual data like emotions and motivations for all the residents in a city is extremely hard. This is where ABM jumps in. Model trained by data sampled in residents of a certain community is able to simulate individual behavior. In this way the simulation of the whole community is achieved and can be validated by the community twin constructed from big data. After the simulation for all the communities are achieved, the integration of all the communities produces the simulation of the whole city that can also be validated by the DT of the city. Once the simulations of each level are validated, they can be deployed and visualized in the DT. Finally, the agents used for ABM are mapped as individual twins of real city residents.

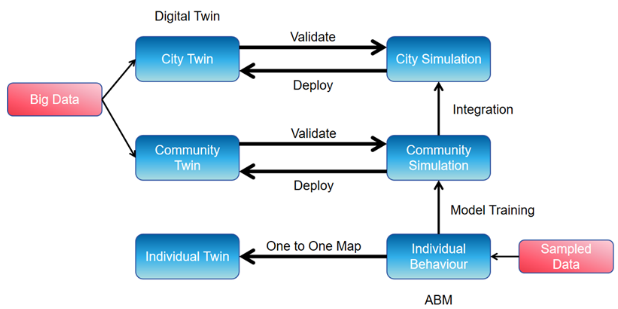

Figure 4: Large scale social simulator integrating ABM and DT in Wuhan, China.

Figure 5 shows the workflow of the LSS. The LSS gathers data from multiple sources. Geographical data is used to construct the environment of identical virtual communities. Macro-level data, such as phone usage and electricity consumption, are employed to train and validate the simulation models. Survey data collected from real residents is used to create AI agents. Detailed road and building information for Wuhan is used to build the DT environment of the city. Real-time big data streams are utilized for validating and calibrating the city-wide real-time simulation. The simulation begins at the community level. AI agents behave according to simulation models trained on macro-level data. Once all AI agents within a given community are trained to behave appropriately, the DT of that community is considered complete. By repeatedly deploying this simulation process across all communities in Wuhan, a real-time simulation of the entire city is generated. Real-time big data streams, such as traffic conditions and population mobility, are then used to further validate and calibrate the simulation. By combining this real-time simulation with detailed spatial data, a high-fidelity DT of Wuhan can be achieved.

4 FUTURE RESEARCH DIRECTIONS

The growing availability of empirical data has increased the focus on data-driven approaches in Agent-Based Modeling and Simulation (ABMS). Technologies like Machine Learning (ML), Large Language Models (LLMs), and Digital Twins (DTs) are increasingly used to leverage this data. For quick reference, Table 1 highlights selected use cases. These examples demonstrate how AI technologies are applied across diverse ABM domains and how different methodologies are integrated. Despite these advancements, significant technical challenges remain, including high computational demands, model interpretability issues, integration complexity, and the need for domain-specific expertise to effectively incorporate these technologies into ABMS.

The use of ML, LLMs, and DT within ABMS requires substantial computational power, for instance, to detect dynamic behavioral changes in large datasets, run an LLM instance for each agent in large-scale simulations, or manage socially complex environments using integrated ABM-DT systems. Further research is needed to address these high computational demands.

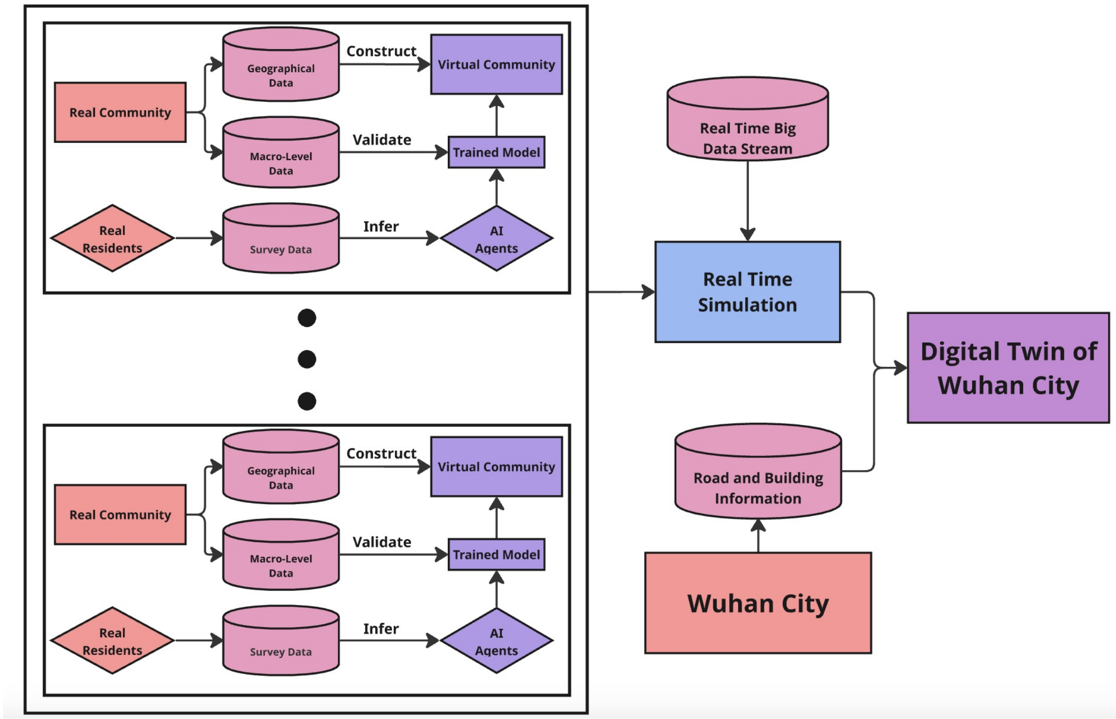

Figure 5: Framework of Real-Time Urban DT: The Case of Wuhan Large-Scale Social Simulator.

Table 1: Representative Applications of AI Integration into ABM.

Application Domain	Specific Applications of ABM with AI Technology
Fire Evacuation (Li et al. 2024)	Deep Reinforcement Learning (DRL) is integrated with Human-Robot Interaction (HRI) to support robot-assisted pedestrian evacuation. By dynamically adjusting robot positions within the fire environment, the model optimizes evacuation paths, alleviates congestion, and enhances overall efficiency.
Public Safety Monitoring (Malleson et al. 2022)	Distributed agent networks incorporate surveillance cameras, IoT sensors, and social media feeds, using machine learning to detect security threats and coordinate real-time police deployment.
Stock Market Simulation (Zhu et al. 2023)	A reinforcement learning framework simulates two types of trading agents—those with and without prior bubble experience—to study decision-making and market fluctuations under heterogeneous behavioral assumptions.
Autonomous Driving (Wachi 2019)	Machine learning transforms scripted traffic simulations into dynamic, data-driven environments. Deep learning models mine human driving datasets to generate realistic background traffic, while closed-loop reinforcement learning identifies and stresses weaknesses in autonomous systems through adversarial scenario generation.
Agricultural Supply Chain (Agricultural 4.0) (Shadkam and Irannezhad 2025)	A conceptual framework combining Digital Twins, Machine Learning, and Agent-Based Modeling enables real-time monitoring, predictive analytics, and scenario testing of agricultural supply chains. This supports adaptive decision-making for efficient and resilient digital agriculture systems.

The integration of ML and LLMs into ABMS can hinder explainability, compounding existing criticisms of model complexity and making simulation outputs harder to interpret. This also complicates validation, especially when ML or LLM components are involved, necessitating further research. Additionally, ABMS studies often risk from over-complexity; incorporating ML, LLMs, and DT may exacerbate this issue. Research is needed to guide appropriate model complexity relative to specific modeling objectives.

AgentBlock.net simplifies integration complexity and technical barriers for non-programmers, enabling a focus on theoretical insights in multidisciplinary research. Its modular repository, containing reusable modules and validation scripts, enhances cross-disciplinary reusability. This design aligns with its goal of making complex system modeling accessible through a modular infrastructure. Thus, it can support future integration with AI, ML, LLMs, and DT modules.

Finally, the non-technical challenges such as ethics and data management are equally important. For example, when building DT of social systems, a large amount of personal and socially sensitive information is involved, requiring strict adherence to ethical principles and legal regulations. This presents a potential challenge for the integration and development of DT and ABM technologies.

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