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# Large language models empowered agent-based modeling and simulation: a survey and perspectives

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Agent-based modeling and simulation have evolved as a powerful tool for modeling complex systems, offering insights into emergent behaviors and interactions among diverse agents. Recently, integrating large language models into agent-based modeling and simulation presents a promising avenue for enhancing simulation capabilities. This paper surveys the landscape of utilizing large language models in agent-based modeling and simulation, discussing their challenges and promising future directions. In this survey, since this is an interdisciplinary field, we first introduce the background of agent-based modeling and simulation and large language model-empowered agents. We then discuss the motivation for applying large language models to agent-based simulation and systematically analyze the challenges in environment perception, human alignment, action generation, and evaluation. Most importantly, we provide a comprehensive overview of the recent works of large language model-empowered agent-based modeling and simulation in multiple scenarios, which can be divided into four domains: cyber, physical, social, and hybrid, covering simulation of both real-world and virtual environments, and how these works address the above challenges. Finally, since this area is new and quickly evolving, we discuss the open problems and promising future directions. We summarize the representative papers along with their code repositories in <https://github.com/tsinghua-fib-lab/LLM-Agent-Based-Modeling-and-Simulation>.

## Introduction

Simulation, as a computational tool, encompasses the emulation of real-world processes or systems by employing mathematical formulas, algorithms, or computer-generated representations to imitate their behaviors or characteristics. Agent-based modeling and simulation focuses on modeling complex systems by simulating individual agents and their interactions within an environment (Macal and North, 2005). It operates by assigning specific behaviors, attributes, and decision-making capabilities to these agents, enabling the examination of emergent phenomena resulting from agents' interactions and environment dynamics. The significance of simulation spans various domains, serving as a valuable tool for understanding, analyzing, and predicting intricate phenomena that might be impractical or impossible to observe directly in real life. It facilitates experimentation, hypothesis testing, and scenario analysis, offering insights into systems' behaviors under diverse conditions and aiding in

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decision-making processes across fields like economics, biology, sociology, and ecology. The capacity to acquire and use language is a key aspect that distinguishes humans from other beings (Hauser et al., 2002). The advent of large language models (LLMs) represents a recent milestone in machine learning, showcasing immense capabilities in natural language processing tasks and textual generation (Zhao et al., 2023). Leveraging their formidable abilities, LLMs have shown promise in enhancing agent-based simulations by enabling more nuanced and realistic representations of agents' decision-making processes, communication, and adaptation within simulated environments. Integrating LLMs into agent-based modeling and simulation holds the potential to enrich the fidelity and complexity of simulations, potentially yielding deeper insights into system-level behaviors and emergent phenomena for the following reasons: First, LLM agents can take actions even if there are no explicit instructions (Team, 2022; Yoheinakajima, 2023). Second, LLM agents can respond like a real human with adaptive planning (Schick et al., 2024; Wang et al., 2024b; Xi et al., 2023). Lastly, LLM agents can interact with other agents (or even real humans) (Park et al., 2023). Thus, LLM agents have achieved success in a lot of areas (Boiko et al., 2023; Bran et al., 2023; Gao et al., 2023; Jinxin et al., 2023; Kovač et al., 2023; Li et al., 2023c, 2023e; Lin et al., 2023; Park et al., 2023, 2022). From this perspective, it is clear that LLM agents can serve as a new paradigm for simulation with human-level intelligence.

As a result of the massive potential of LLM agents, there has recently been a boom in research efforts in this area. However, as yet, there is no survey that systematically summarizes the relevant works, discusses the unresolved issues, and provides a glimpse into important research directions. In this survey, we analyze why large language models are essential in the fundamental problem of simulation, especially for agent-based simulation. After discussing how to design agents in this new paradigm, we carefully and extensively discuss and introduce the existing works in various areas, most of which have been published recently. The contribution of this survey can be summarized as follows.

- We take the first step to review the existing works of large language model-based agent modeling and simulation. We systematically analyze why large language models can serve as an advanced solution for agent-based modeling and simulation compared with existing approaches. Specifically, we first extensively explain the requirements of the agent capability for agent-based modeling and simulation from four aspects: autonomy, social ability, reactivity, and pro-activeness. Then, we analyze how large language models address these challenges, including perception, reasoning and decision-making, adaptivity, and heterogeneity.
- We divide the agent-based modeling and simulation into four domains, physical, cyber, social, and hybrid, which can cover the mainstream simulation scenarios and tasks, after which we present the relevant works, providing a detailed discussion about how to design the simulation environment and how to build simulation agents driven by large language models.
- In addition to the existing works in this new area, we discuss four important research directions, including improving the simulation of scaling up, open simulation platform, robustness, ethical risks, etc., which we believe will inspire future research.

**Discussions on PRISMA.** Following Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA), we provide more details of how we collect and organize the related

works. (1) *Eligibility criteria, Information sources, and Search strategy.* For the eligibility criteria, we delineate the scope of the review, including (1) the usage of LLM agents and (2) the studied problem of agent-based modeling and simulation. Information sources for our paper are diverse, encompassing peer-reviewed journals, conference proceedings, preprint archives, and reputable databases like IEEE Xplore, ACM Digital Library, Elsevier, Clarivate Web of Science, arXiv preprint, SSRN preprint, etc. The search strategy we used incorporates a combination of keyword searches and controlled vocabulary terms related to LLMs, ABMS, and their intersection, of which the keywords include “large language models,” “agent-based simulation,” “intelligent agents,” “AI-driven simulation,” etc. We also use the citation tracking function of Google Scholar to identify cited/citing papers for those seminal works, ensuring a thorough and relevant literature review. We believe this structured approach will facilitate a comprehensive understanding of the current landscape and emerging trends using LLM agents for ABMS. (2) *Selection process, Data collection process, and Data items.* After deploying the search strategy on the various information sources, we select the proper papers presented in this review. The filtering process mainly focuses on two specific problems: (1) double-checking whether the paper belongs to agent-based modeling simulation and uses LLM agents and (2) what kind of sub-category this paper belongs to. For the first problem, we found some papers that use an LLM agent as an assistant or decision-making helper, which is close to agent-based modeling and simulation but, indeed, not the same. We filter out these papers (20+) and reserve the remaining ones. For the second problem, we categorize the papers based on two-dimension criteria: the domain and the environment.

## Background

In this section, we will first introduce the background of agent-based modeling and simulation, and large language models-empowered agents.

### Agent-based simulation

*Basic concepts of agent-based simulation.* Agent-based simulation captures the intricate dynamics inherent in complex systems by concentrating on individual entities referred to as agents (Macal and North, 2005). These agents are heterogeneous, with specific characteristics and states, and adaptively behave according to context and environment, making decisions and taking actions (Elsenbroich et al., 2014). The environment, whether static or evolving, introduces conditions, instigates competition, defines boundaries, and occasionally supplies resources influencing agent behaviors (Cipi and Cico, 2011). The interaction includes interactions with both the environment and other agents, and the goal is to mirror the behaviors in reality based on predefined or adaptive rules (Elliott and Kiel, 2002; Macal and North, 2005). To summarize, the basic components of agent-based simulation include:

**Agents:** Agents are the fundamental entities in an agent-based simulation. They represent individuals, entities, or elements in the system being modeled. Each agent has its own set of attributes, behaviors, and decision-making processes.

**Environment:** The environment is the space in which agents operate and interact. It includes the physical space, as well as any external factors, e.g., weather conditions, economic changes, political shifts, and natural disasters, that influence agent behavior. Agents may be constrained or influenced by the

environment, and their interactions can have effects on the environment itself.

**Interaction:** Agents interact with each other and their environment through predefined mechanisms. Interactions can be direct (agent-to-agent) or indirect (agent-to-environment or environment-to-agent).

With the above components, agent-based modeling and simulation provide a bottom-up perspective to study the macro-level phenomena and dynamics from the individual interactions.

**Agent capability.** To achieve realistic simulation in a wide range of application domains, agents should have the following capabilities in terms of perception, decision, and action (Wooldridge and Jennings, 1995).

**Autonomy:** Agents should be able to operate without the direct intervention of humans or others, which is important in real-world applications such as microscopic traffic flow simulation (Lopez et al., 2018) and pedestrian movement simulation (Batty, 2001).

**Social ability:** Agents should be able to interact with other agents (and possibly humans) to complete the assigned goals. When studying social phenomena, group behavior, or social structures, the sociability of agents is key. This includes simulating the formation of social networks, the dynamics of opinions, the spread of culture, and more. The social interactions between agents can be either cooperative or competitive, which are critical when simulating economic activities such as market behavior, consumer decisions, etc.

**Reactivity:** Agents should be able to perceive their environment and respond quickly to changes in the environment. This capability is especially important in systems that need to simulate real-time responses, such as traffic control systems and automated production lines, and in disaster response scenarios where agents need to be able to respond to environmental changes immediately to effectively conduct early warning and evacuation. More importantly, agents should be able to learn from previous experience and adaptively improve their responses, similar to the idea of reinforcement learning (Lin, 1992).

**Pro-activeness:** Agents should be able to exhibit goal-directed behavior by taking the initiative instead of just responding to their environment. For example, agents need to proactively provide help, advice, and information in applications such as intelligent assistants and actively explore their environment, plan paths, and perform tasks in fields such as autonomous robots and self-driving cars.

It is worth mentioning that, like humans, agents cannot make perfectly rational choices due to limitations of knowledge and computational capacity (Simon, 1997). Instead, they can make suboptimal yet acceptable decisions based on imperfect information. This capability is particularly critical in achieving human-like simulations in the economic market (Arthur, 1991) and management organizations (Puranam et al., 2015). For example, considering agents' bounded rationality when simulating consumer behavior, market transactions, and business decisions can more accurately reflect real economic activities. In addition, in simulating decision-making, teamwork, and leadership within organizations, bounded rationality helps reveal behavioral dynamics in real work settings.

**Applications of agent-based modeling and simulation.** The flexibility of agent-based modeling and simulation allows for the

exploration of diverse scenarios and the study of emergent phenomena in a controlled simulation environment. Therefore, it offers researchers and practitioners a versatile tool for understanding and predicting the behavior of complex systems across various domains.

Based on the four categories of the target systems, current works of agent-based simulation can be divided into four domains.

**Physical domain:** This category refers to the natural system in the physical environment (An, 2012). Typical applications include *ecology and biology* (Pereira et al., 2004; Zhang and DeAngelis, 2020), such as modeling ecological systems (Heckbert et al., 2010; Lippe et al., 2019), species interactions (McLane et al. (2011), and the impact of environmental changes (Beltran et al., 2017; Pertoldi and Topping, 2004). Many simulation problems in urban environments also belong to the physical domain (An, 2012), such as transportation, human mobility, etc. Specifically, for urban planning (Gaube and Remesch, 2013), agent-based modeling and simulation can aid in simulating urban growth (Arsanjani et al., 2013; Barros, 2004), traffic patterns (de Souza et al., 2019; Mastio et al., 2018), and the impact of urban policies (Ma et al., 2013; Maggi and Vallino, 2016; Widener et al., 2013). Another application is *engineering and manufacturing* (Barbosa and Leitão, 2011; Rolón and Martínez, 2012), in which agent-based modeling and simulation can be applied to model supply chain dynamics (Schieritz and Grobler, 2003), production processes (Parv et al., 2019), and the interactions of entities within manufacturing systems.

**Social domain:** The social domain mainly covers the social behavior simulation, which can be further divided into (1) social interaction that focuses on social networks, community interactions, or organizational behavior (Macy and Willer, 2002; Wall, 2016) and (2) economic system that simulates economic systems, market dynamics, or financial interactions (Samanidou et al., 2007). Specifically, for social sciences (Conte and Paolucci, 2014; Gilbert, 2007b; Gilbert and Terna, 2000; Terna et al., 1998), agent-based modeling and simulation are widely used to model social phenomena such as crowd behavior (Kountouriotis et al., 2014; Luo et al., 2008), opinion dynamics (Banisch et al., 2012; Li et al., 2020), and social network interactions (El-Sayed et al., 2012; Gilbert, 2004a; Madey et al., 2003). The agent-based modeling can simulate the emergence of societal patterns and trends (Helbing, 2012). As for the research of economics (Hamill and Gilbert, 2015; Leombruni and Richiardi, 2005; Van Dinther, 2008), agent-based models are employed to study economic systems (Deguchi, 2011), market dynamics (Rouchier, 2017; Wang et al., 2018), and the behavior of individual economic agents (Mueller and Pyka, 2016).

**Cyber domain:** Besides the physical world and human society, our daily life has been further extended into cyberspace. Therefore, agent-based simulation has also been applied in wide areas like web-based behaviors (Guyot and Honiden, 2006) and cybersecurity applications (Alluhaybi et al., 2019).

**Hybrid domain:** This category includes hybrid systems combining components covering the physical world, social life, and cyberspace. For example, an urban environment is a socio-physical environment that integrates social behavior with physical infrastructure. Moreover, it is also multi-layered after taking online social networks into account. That is, these applications involve more than one domain of physical, social, or cyber domains. Therefore, agent-based simulations within an urban environment, such as urban planning (Chen, 2012) and epidemic control (Silva et al., 2020), are far more complex and challenging than those in unitary environments. Moreover, for *healthcare* (Barnes et al.,

2013; Cabrera et al., 2011), agent-based modeling and simulation can be used to model the spread of infectious diseases (Perez and Dragicevic, 2009), healthcare systems (Silverman et al., 2015), and the effectiveness of interventions (Beheshti et al., 2017), which help in understanding and planning for public health scenarios.

*Methodologies of agent-based modeling and simulation.* The development of modeling technologies utilized in agent-based simulation has also gone through the early stage of knowledge-driven approaches and the recent stage of data-driven approaches. Specifically, the former includes various approaches based on predefined rules or symbolic equations, and the latter includes stochastic models and machine learning models.

- *Predefined rules:* This approach involves defining explicit rules that govern agent behaviors. These rules are typically based on logical or conditional statements that dictate how agents react to specific situations or inputs. The most well-known example is the cellular automata (Wolfram, 1984) that leverages simple, local rules to simulate complex global phenomena that exist not only in the natural world but also in complex urban systems.
- *Symbolic equations:* Compared with predefined rules, symbolic equations are used to represent relationships or behaviors in a more formal, mathematical manner. These can include algebraic equations, differential equations, or other mathematical formulations. A typical example is the social force model widely used in pedestrian movement simulation (Helbing and Molnar, 1995). It assumes that pedestrian movements are driven by a Newton-like law decided by an attractive force driven by the destination and a repulsive force from neighboring pedestrians or obstacles.
- *Stochastic modeling:* This approach introduces randomness and probability into agent decision-making, which is useful for capturing the uncertainty and variability inherent in many real-world systems (Feng et al., 2012). For example, to account for the impact of randomness originating from human decision-making, we can leverage discrete choice models for simulating pedestrian walking behaviors (Antonini et al., 2006).
- *Machine learning models:* Machine learning models allow agents to learn from data or through interaction with their environment. Supervised learning approaches are generally used for estimating parameters of agent-based models, while reinforcement learning approaches are widely used in the simulation period, enhancing the adaptation capability of agents within dynamic environments (Kavak et al., 2018; Kim et al., 2021; Platas-López et al., 2023).

*Limitations.* Early works on agent-based simulation are keen to design “deliberative architectures” that rely on explicit, often complex, internal models to make decisions, emphasizing the importance of planning, reasoning, and decision-making processes (Wooldridge and Jennings, 1995). However, optimizing the internal world model and planning-reasoning module based on symbolical AI approaches are generally intractable in practice. This leads to the prevalence of “reactive architectures” in agent-based simulations, which instead rely primarily on direct sense-action loops rather than complex internal models of the world or deep reasoning processes to make decisions. The subsequent development of AI, especially deep learning technology, does not fundamentally change this paradigm of agent-based simulation due to the poor interpretability and generalization capability. However, facing the need for realistic simulation of real-world processes or systems, current approaches still have several limitations, as described below.

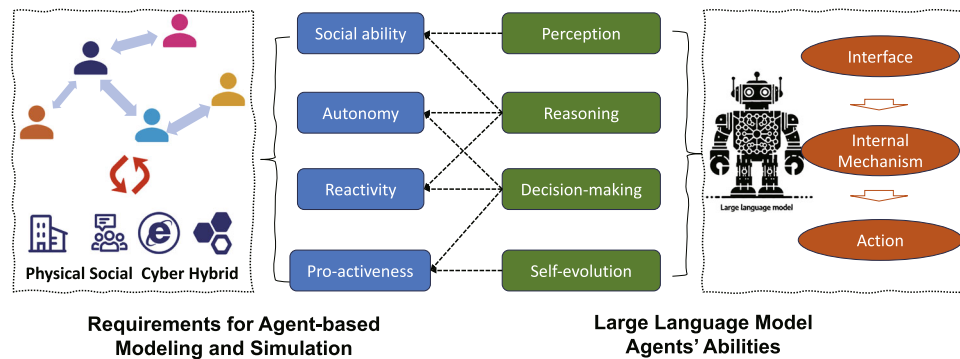
Simple agent architecture is not enough to cope with complex tasks: Although “reactive architectures” are able to adapt to different environmental conditions, they may be limited in handling complex tasks or situations that require long-term planning. To achieve human-like simulation in real-world complex problems, current agent architecture requires redesigns that solve challenges in processing speed, resource efficiency, and task complexity. Specifically, agents should be capable of complex planning and reasoning processes, like using internal models to predict the consequences of different courses of action and choose the best one, and able to develop and execute complex strategies to achieve long-term goals.

It is difficult to develop a general agent that can support simulations across environments: Different environments vary in dimensions like complexity, dynamics, and uncertainty. Due to this diversity, a specific agent that is effective in one environment (like a financial market simulation) might be completely ineffective in another (like a social campaign simulation). In real-world applications where the target environment is often hybrid with significant dynamics and uncertainty, developing specific agents case by case is highly inefficient and costly.

Existing methods cannot support integrative simulation in real-world problems: A versatile agent-based simulation model should be able to describe how systems operate under known conditions, explain why certain patterns emerge, predict future states based on existing observations, and explore the outcomes of hypothetical scenarios. However, existing methods cannot support the above tasks simultaneously: rule-based methods are useful in descriptive problems, while symbolic or stochastic methods can provide explanations regarding underlying mechanisms that drive the system. Comparatively, machine learning models are better at predictive problems by learning hidden patterns from data but with less interpretability. Therefore, there remain challenges in developing methods that simultaneously capture the accuracy of behavioral modeling, interpretability of mechanisms, adaptability, and reliability under environmental changes.

**Large language models and LLM-empowered agents.** Large language models (LLMs), such as ChatGPT (OpenAI, 2022), Gemini (DeepMind, 2023), LLaMA (Touvron et al., 2023), Alpaca (Taori et al., 2023), and GLM (Zeng et al., 2023), are the latest paradigm of language models, which evolve from early statistical language models (Bellegarda, 2004) to neural language models (Melis et al., 2017), then to pre-trained language models (Brown et al., 2020), and finally to large language models (Zhao et al., 2023c). With billions of parameters and extensive pre-training corpus, LLMs have shown astonishing abilities not only in natural language processing tasks (Li et al., 2023a; Zhang et al., 2024c) such as text generation, summarization, translation, etc., but also in complex reasoning and planning tasks, such as solving mathematical problems (Arora et al., 2023), etc. Pre-training on large-scale corpora lays the foundation ability for zero-shot generalization. Moreover, pre-trained models can be further fine-tuned for specific tasks, adapting to particular application scenarios (Jiang et al., 2023). In addition, the advances of large language models in the past year, such as ChatGPT and GPT-4 have achieved human-like reasoning ability, a milestone that is now being considered to be the seed of artificial general intelligence (AGI). Specifically, the capacity to acquire and use language is a key aspect of how we humans distinguish ourselves from other beings (Tomasello, 2010). Language is one of the most important mechanisms we have to interact with the environment, and





**Fig. 1** Illustration of how large language model agents meet the requirements of agent-based modeling and simulation.

language provides the basis for high-level abilities (Hauser et al., 2002).

Thus, it is promising to construct large language model-empowered agents (Wang et al., 2024b; Xi et al., 2023) due to their human-like intelligence in perceiving the environment and making decisions. In the following, we have a short summary of the motivations to apply large language models to agent-based modeling and simulation.

First, the LLM agent is able to adaptively react and perform tasks based on the environment without predefined explicit instructions (Team, 2022; Yoheinakajima, 2023). In addition, during the simulation process, the LLM agent can even form new ideas, solutions, goals, etc. (Franceschelli and Musolesi, 2023). For example, AutoGPT Team (2022) can automatically schedule plans when given a set of available tools and the final task goal, exemplifying the significant potential of LLMs in constructing autonomous agents. Meanwhile, BabyAGI (Yoheinakajima, 2023) created an LLM-driven script running an infinite loop, which continuously maintains a task list, in which each task is completed the task by ChatGPT API (OpenAI, 2022) based on the task context. Second, the LLM agent has enough intelligence that it can respond like a human and even actively take actions with self-oriented planning and scheduling (Wang et al., 2024b; Xi et al., 2023). Actually, the input of the environment is not limited to text; rather, recent multi-modal fusion models can be fed other types of information, such as image or audio (Zhu et al., 2024). The action space of the LLM agent is neither limited to text, for which the tool-usage ability allows the agent to take more actions (Schick et al., 2024). Third, the LLM agent has the ability to interact and communicate with humans or other AI agents (Park et al., 2023). In the simulation, especially agent-based simulation, the agent's communication ability elevates individual simulation to the community level (Gilbert and Troitzsch, 2005). An LLM-driven agent can generate text, which can be received and understood by another agent, in turn providing the basis for interpretable communication among agents or between humans and agents (Park et al., 2023). Fourth, the simulation at the community level requires heterogeneity of agents, and the LLM agents can meet these requirements for playing different roles in society (Qian et al., 2024). An artificial society constructed by LLM agents can further reveal the emergence of swarm intelligence with collective agent behaviors (Gao et al., 2023; Park et al., 2023), similar to wisdom-of-crowds in human society (Surowiecki, 2005).

As mentioned above, the simulation system has widely utilized the paradigm of agent-based modeling, which requires agents with high-level abilities. This well motivates the use of large language model-empowered agents in simulation scenarios. In the following, we will discuss the critical abilities of a large language model for agent-based modeling and simulation in

detail in the section "Critical abilities of LLM for agent-based modeling and simulation". Then, in the section "challenges and approaches of LLM agent-based modeling and simulation", we will elaborate on the recent advances of large language model agent-based modeling and simulation to further answer the question of how large language model agents meet the requirements (what kind of challenges and how to address them).

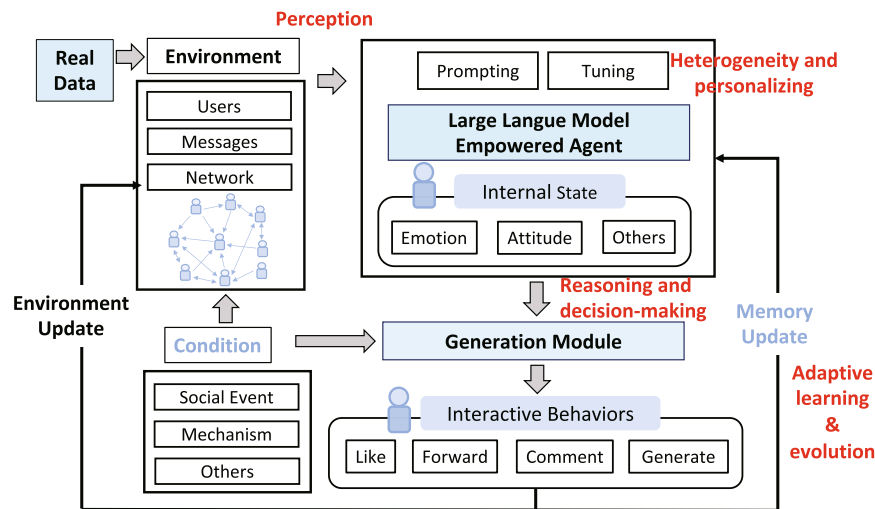
### Critical abilities of LLM for agent-based modeling and simulation

As mentioned above, agent-based modeling and simulation serve as a basic approach for simulation in many areas (Elsenbroich et al., 2014; Macal and North, 2005), but it still suffers from several key challenges. Large language model-empowered agents not only meet the requirements for agent-based simulation but also address the limitations relying on their strong abilities in perception, reasoning, decision-making, and self-evolution, illustrated in Figs. 1, 2.

**Perception.** The core of agent-based modeling and simulation is to model how an individual agent interacts with an environment (Macal and North, 2005), which requires the agent to accurately sense various types of information from said environment. As for the large language model-empowered agents, the ability of language enables agents to comprehend and respond to diverse environments directly or indirectly. On the one hand, the basic ability to understand and generate text enables agents to engage in complex dialogs, negotiate, and exchange information, and support direct interaction. On the other hand, the interface between the agent and environment can be operated via texts (Team, 2024), which leads to indirect interaction. Of course, such ability also supports the communication between different agents, besides the agent-environment perspective.

It is worth mentioning that the ability to interact with the environment and other agents is not adequate to achieve human-like simulations. To be more specific, it is also required that large language model-based agents "put themselves in real humans' shoes", thereby allowing the agent to imagine that it is *indeed in the environment*. That is, LLM agents should be able to comprehend, perceive, and respond to diverse needs, emotions, and attitudes within different contexts, from the "first-view sight" (Shanahan et al., 2023). This capability enables models to better understand the information from the environment or other agents and generate more real responses.

**Reasoning and decision making.** One critical challenge in traditional agent-based simulation is that rule-based or even neural network-based agents is *not intelligent enough* (Cipi and Cico, 2011). That is, the agent is not able to make correct or optimal



**Fig. 2** Illustration of how large language model-empowered agents work based on four aspects of critical abilities (figure edited from S3 Gao et al., 2023): perception, heterogeneity and personalizing, reasoning and decision-making, adaptive learning, and evolution.

decisions, such as choosing a crowded road in the transportation simulation or sending an incorrect message in the social network simulation. This can be explained by the fact that traditional neural network-based artificial intelligence is still not as intelligent as a real human (Hernández-Orallo et al., 2016; Hoshen and Werman, 2017; Liu et al., 2019; Mańdziuk and Żychowski, 2019). In contrast, large language model-empowered agents exhibit heightened reasoning capabilities, enabling them to make more informed decisions and choose suitable actions within the simulation. Despite making suitable decisions, another critical advantage of large language model-empowered agents to support better agent-based modeling and simulation is autonomy (Fu et al., 2024). With only limited guidance, regulations, and goals, agents equipped with large language models can autonomously take actions, make plans for the given goal, or even achieve new goals without the need for explicit programming or predefined rules (Park et al., 2023). That is, autonomy enables LLM agents to dynamically adjust their actions and strategies based on real circumstances, contributing to the realism of the simulation.

**Adaptive learning and evolution.** For agent-based modeling and simulation, the system always has uncertainty and controllability (Macal and North, 2005). In other words, the environment and the agent's state may be completely different compared with the initial stage of the simulation. As the old story of *Rip Van Winkle* tells, a man falls asleep in the mountains and awakens to find that the world around him has drastically changed during his slumber. That is, the environment is continuously changing in a long-term social network simulation (Gao et al., 2023); the agent should be able to adapt to the new environment, formulating decision policies that may deviate significantly from their original strategies. Obviously, adaptive learning and evolution are challenging for traditional approaches, but luckily, this can be addressed by large language model-based agents (Lu et al., 2023). Specifically, with the ability to continually learn from new data and adapt to changing contexts, LLM agents can evolve behaviors and decision-making strategies over time. Agents can assimilate new information, analyze emerging patterns in data, and modify their responses or actions accordingly based on in-context learning (Dong et al., 2022), mirroring the dynamic nature of real-world entities. This adaptability contributes to the simulation's realism by simulating the learning curve and evolution of agents' behaviors in response to varying stimuli.

**Heterogeneity and personalizing.** As the saying goes, *one man's meat is another man's poison*. Heterogeneity of agents is critical for agent-based simulation, with the complex society (Brown and Robinson, 2006) or economic system (Bohmann et al., 2010) with heterogeneous individuals. Specifically, in agent-based modeling and simulations, the heterogeneity of agents involves representing diverse characteristics, behaviors, and decision-making processes among individuals. Agent-based simulation stands out for its capacity to accommodate varied rules or parameters compared to traditional simulation methods, discussed as follows.

The first one is the extremely high complexity of parameter settings of the existing methods (Elliott and Kiel, 2002; Macal and North, 2005). In these models, the vast array of variables influencing an agent's behavior—from personal traits to environmental factors—makes selecting and calibrating these parameters daunting. This complexity often leads to oversimplification, compromising the simulation's accuracy in portraying true heterogeneity (Macal and North, 2005). Moreover, acquiring accurate and comprehensive data to inform parameter selection is another challenge. That is, real-world data capturing diverse individual behaviors across various contexts might be limited or challenging to collect. Furthermore, validating the chosen parameters against real-world observations to ensure their reliability adds another layer of complexity. Second, the rule or the model cannot cover all dimensions of heterogeneity, as real-world individuals are very complex (Macal and North, 2005). Using rules to drive agent behaviors only captures certain aspects of heterogeneity but could lack the depth to encapsulate the full spectrum of diverse behaviors, preferences, and decision-making processes. Furthermore, as the model capacity, trying to cover all dimensions of heterogeneity within a single model is too idealistic. Thus, balancing model simplicity and accurate modeling agents becomes a critical challenge in agent-based modeling and simulation, resulting in oversimplification or neglect of certain aspects of agent heterogeneity.

Different from the traditional methods, the LLM-based agents support (1) capturing complex internal characteristics with internal human-like cognitive complexity and (2) specialized and customized characteristics with prompting, in-context learning, or fine-tuning.

*An example of a better understanding.* For a better understanding of the above abilities of large language model agents, we select the paradigm of a representative paper, S3 in the social domain, as a

template and add more supplementary descriptions to construct a representative diagram. We have done some editing on the original figure, and the improved figure illustrates a representative agent workflow that reveals four critical abilities: perception, heterogeneity and personalizing, reasoning and decision-making, adaptive learning, and evolution. The overall structure is also very similar to Generative Agent (Park et al., 2023).

### Challenges and approaches of LLM agent-based modeling and simulation

The core of agent-based modeling and simulation is how the agent reacts to the environment and how agents interact with each other, in which agents should behave close to real-world individuals with human knowledge and rules, as real as possible. Therefore, when constructing large language model-empowered agents for simulation, there are four major challenges, including perceiving the environment, aligning with human knowledge and rules, choosing suitable actions, and evaluating the simulation. We will discuss the solutions from a high-level perspective, and how the existing works address them will be elaborated on in detail in the next section.

**Environment construction and interface.** For agent-based simulation with large language models, the first step is to construct the environment, virtual or real, and then design how the agent interacts with the environment and other agents. Thus, we need to propose proper methods for an environment that LLM can perceive and interact with.

*Environment: define the world and rules.* The external environment in agent-based simulation varies for different domains. In general, the environment built by existing works can be divided into two categories: virtual and real.

- The virtual environment includes simulation applications with predefined rules in prototype-level simulation, such as a virtual social system, game, etc. For example, Qian et al. (2024) designed a virtual software company with multiple agents for different roles, such as CEO, managers, programmers, etc. Wang et al. (2023b) constructed an environment of a virtual recommender system in which agents can browse the recommended contents and provide feedback. The sandbox environment is one kind of virtual environment where the principles and ideas conceptualized in a virtual environment can be tested and adapted to real-world applications. For example, Generative Agent Park et al. (2023) builds a Smallville sandbox world in which large language model-empowered agents plan their days, share news, form relationships, and coordinate group activities.
- The real environment includes our real world. For example, Li et al. (2024b) deploy large language model-based agents to simulate economic activities, in which agents can represent both consumers and workers. WebAgent Gur et al. (2024) simulate a real human browsing and accessing online content of real websites. UGI (Xu et al., 2023a) proposed to build agents for the real-world urban environment, and the agents are expected to generate various human behaviors in the city, including navigation, social, economic, etc.

*Interface.* The interface actually has two aspects, how the agent interacts with the environment and how agents communicate with each other.

- Input and output of the environment. Most existing works use texts as the major interface, naturally due to the ability to understand and generate texts of large language models. Even if the environment is a sandbox with rich models, such as Smallville sandbox world (Park et al., 2023) in which the environment is still represented with texts, relying on which the agent can perceive the context. In addition, the basic rules or domain-specific knowledge, such as the game rule, is also summarized with texts, which are received by the large language model agents with prompt engineering. Due to the limitation of texts, the existing works construct various tools to interact with complex environments or data, but recalling or using these tools is still based on texts. For example, in Zhu et al. (2023c), the large language model's action is a phrase, which can be a parameter of the tool function to interact with the simulation environment.
- Communication between agents. First, the direct communication between agents is also focusing on the texts. For example, in agent-based simulation for social science, the textual information exchange represents the communication between humans in the real world. Second, the agents can indirectly interact with others through predefined rules; for example, in economic simulation, the agents can work in the same factory, and the rule in the economic system makes them interact indirectly.

In summary, the environment construction, along with defining how agents interact with the environment, is the first step of deploying large language model agents for agent-based modeling and simulation. Thanks to the multi-modal ability and usage of tools, the interface is not limited to pure texts, supporting more diverse and more realistic environments, with more complicated cross-agent interactions.

**Human alignment and personalization.** Although LLMs have already demonstrated remarkable human-like characteristics in many aspects, agents based on LLMs still lack the necessary domain knowledge in specific areas, leading to irrational decisions. Therefore, aligning LLM agents with human knowledge and values, especially those of domain experts, is an essential challenge to achieve more realistic domain simulations. However, the heterogeneity of agents, as a fundamental characteristic of ABM, is both an advantage and a challenge for traditional models. While, LLMs possess a powerful capability to simulate heterogeneous agents, ensuring controllable heterogeneity. However, enabling LLMs to play different roles to meet personalized simulation requirements is a significant challenge. Next, we will explain the methods and technologies to address these two challenges from two perspectives: prompt engineering and tuning, and introduce the existing related work in these areas.

#### Human alignment

*Prompt engineering:* When simulating specific agents, we can provide task instructions, background knowledge, generation patterns, and task examples specific to certain domains or scenarios, thereby aligning LLMs' output with human knowledge and values when deployed. For example, providing detailed descriptions of game rules and examples for the agent allows it to consider various factors it cares about, like humans when making decisions, such as self-interests, fairness, etc. (Akata et al., 2023). In addition, constructing modules such as reflection and memory can improve agents' planning and reasoning capabilities, thereby giving them stronger gaming capabilities and creating a possible path towards human-intelligent gaming (Guo et al., 2023).



**Tuning:** Tuning requires constructing a training dataset for specific domains, scenarios, or hiring domain experts. Based on the dataset or expert feedback, fine-tuning the LLM can also empower the agents with more domain-specific knowledge, producing outputs more in line with human knowledge and values. For example, Singhal et al. (2023) propose to achieve knowledge alignment in clinical medicine. The proposed Multi-MedQA benchmark combines six existing medical question-and-answer datasets covering professional medicine, research, and consumer inquiries. Additionally, Med-PaLM (Singhal et al., 2023), an LLM for the medical field, is trained based on a foundational model PaLM (Chowdhery et al., 2023). In terms of implementation, the authors incorporate examples of medical question-and-answer and modify model prompts through the guidance of professional clinicians (involving five clinical doctors) for fine-tuning. This guides the model to generate text consistent with clinical requirements. With this domain-specific LLM, we can simulate agents (e.g., medical assistants) in real-world medical environments. In addition to collecting large-scale datasets with domain knowledge, other research (Dubois et al., 2024) directly uses LLMs to generate “human feedback”, specifically pair-wise feedback for instructions, for LLM fine-tuning. Results show that the generated feedback enables LLM to achieve high human alignment 45× cheaper than hiring crowd workers to give feedback in experiments.

#### *Personalization*

**Prompt engineering:** The basic idea is to adapt to personalized needs by providing LLM agents with individual preferences, expected output patterns, background knowledge, etc., thereby making the output closer to the specific needs or preferences of individuals when deployed. For example, in the well-known LLM-based social activity simulation, AI Town (Park et al., 2023), personalized interaction behaviors of agents in different scenarios, at different times, and with different other agents can be achieved by introducing professions, behavioral preferences, and interpersonal relationships in the prompts. In economic simulation, specifically the simulation of canonical games, the agent’s preferences can be specified in the prompt, such as cooperative, selfish, altruistic, etc., so that the agent will have different levels of cooperative tendencies during the game playing (Phelps and Russell, 2023).

**Tuning:** Tuning for personalization requires selectively constructing datasets or fine-tuning multiple models based on feedback from different users, with each model corresponding to one or a type of personalized needs. This can also be achieved by using specific combinations to provide relevant, personalized requirements. Some research attempts to efficiently align LLMs with various preferences tailored to different users’ distinct preferences (Jang et al., 2023). Specifically, user preferences are decomposed into standards across multiple aspects, with personalized optimization based on RLHF targeted towards different aspects. In practical applications, the strategy of LLM response generation is based on linearly weighting strategies according to user preferences. When simulating agents with individual preferences (e.g., users in recommender systems), this approach achieves a more accurate match for different preferences and is also easily generalizable to scenarios with a broader range of preferences.

In summary, human alignment and personalization ensure the large language model-empowered agents cannot only simulate real human behaviors but also play a given role, making it possible to simulate the heterogeneity of real-world systems. The typical techniques in this component mainly involve prompt engineering and tuning.

**How to simulate actions.** This section aims to delve into how LLM agents are designed to exhibit complex behaviors that are reflective of real-world cognitive processes. This involves understanding and implementing the mechanisms by which these artificial agents can retain and utilize past experiences (memory) (Gao et al., 2023; Park et al., 2023; Zhu et al., 2023c), introspect and adjust their behavior based on their outcomes (reflection) (Park et al., 2023; Shinn et al., 2023), and execute a sequence of interconnected tasks that mimic human workflows (planning) (Wei et al., 2022).

**Planning.** Here, we introduce the methodology by which LLM agents approach complex tasks through decomposition. Initially, an LLM assesses the task to understand its main objectives and context. It then breaks down the task into smaller, manageable subtasks, each contributing towards the overall goal. This segmentation leverages the LLM’s training corpus to recognize patterns and apply relevant knowledge efficiently (Park et al., 2023; Sun et al., 2024); Wang et al., 2024a; Zhu et al., 2023c).

Each subtask is executed sequentially, with the LLM agent applying its knowledge base to ensure logical progression and coherence. This approach not only simplifies complex tasks but also enhances the LLM’s accuracy and adaptability. By tackling tasks incrementally, the LLM agent can adapt its strategies and ensure that each step is contextually relevant and logically structured. For example, GITM (Zhu et al., 2023c) showcase an LLM agent that decomposes the overarching goal of “Mining Diamond” into a series of sub-goals, constructing a sub-goal tree. This model uses its text-based knowledge and memory to navigate in a virtual environment, making strategic decisions at each tree node to achieve the main objective. Voyager Wang et al. (2024a) employ an automatic curriculum to aid the LLM agent in understanding the sequence of actions required to reach a goal. By reasoning with the available resources, the LLM agent can plan an efficient course of action, like upgrading tools for better efficacy and demonstrating adaptive problem-solving skills. AdaPlanner (Sun et al., 2024) introduces an LLM that refines its action plan based on feedback, which has an in-plan refiner for aligning actions with predictions and an out-of-plan refiner to adjust when predictions do not match outcomes, showcasing the model’s ability to adapt and revise its plan dynamically in response to changing scenarios.

In summary, advancements represent significant strides in task decomposition and strategic planning. They highlight the capability of LLMs to not only break down complex tasks into manageable sub-goals but also to dynamically adapt their strategies and refine plans based on ongoing feedback and changing scenarios, thereby enhancing decision-making and problem-solving efficiency in various contexts.

**Memory.** Human behavior is largely influenced by past experiences and insights, which are stored in memory. If LLM agents aim to mimic this aspect of human behavior, they also need to reference past experiences and insights when acting. However, the volume of this information is often immense, frequently exceeding the context window length of LLMs. Therefore, it’s necessary to design a memory system that functions as an external database for LLM agents. This system should have appropriate mechanisms for organizing, updating, and retrieving information, enabling LLM agents to reference these memories for future actions.

Generative Agents Park et al. (2023) showcase an LLM agent that develops a generative memory system, integrating sensory perceptions with a continuous stream of experiences. This system not only stores information but actively engages in planning and reflection, adapting its behavior based on past outcomes. Chen



et al. (2023c) illustrate an LLM agent's strategic prowess in auction scenarios, where it adapts its bidding strategy by synthesizing new information with existing memories to maximize profits or meet specific objectives.

GITM (Zhu et al., 2023c) and Voyager (Wang et al., 2024a) are seen curating a skill library, updating its capabilities through practice and feedback. This approach reflects an understanding of task requirements and environmental challenges, where the LLM's memory serves as a dynamic repository of actions and strategies. The distinction between explicit and implicit memory comes into play in simulations that require the LLM to navigate complex tasks, such as resource management and goal-oriented action planning in open-world environments. Here, the LLM's memory functions extend beyond simple recall, enabling the agent to perform with a sense of history and progression.

Lastly, the role of memory in social interactions is explored through simulations in S3 (Gao et al., 2023) that mimic the intricacies of human behavior. LLMs track and adapt to changing social cues and demographic shifts, employing memory not just as a record of past interactions but as a tool for future social navigation and decision-making. Li et al. (2024b) demonstrate how a memory module in LLMs can be crucial for understanding and adapting to dynamic social environments. They show that LLMs, equipped with a memory of past social interactions and trends, can more effectively predict and respond to future economic changes, enhancing their decision-making in complex social landscapes.

Collectively, these studies contribute to our understanding of LLMs as agents capable of sophisticated memory management, crucial for their function in dynamic and unpredictable environments. They highlight the remarkable potential of LLMs to transcend traditional data storage, moving towards a more integrated and intelligent use of memory in artificial cognition.

**Reflection.** The section explores how LLM agents incorporate feedback mechanisms to enhance their memory systems, improving decision-making and learning processes. This reflection encompasses both short-term and long-term memory facets, enabling LLMs to adapt their behaviors and strategies dynamically.

An exemplary implementation of this reflective cycle is Reflexion (Shinn et al., 2023). In this work, the LLM leverages an integrated evaluator to internally assess the efficacy of actions based on the rewards received. It also utilizes a prompt-based approach to self-reflection, allowing the agent to internally simulate and critique its performance. This dual feedback system enables the agent to refine its memory and behavior in a nuanced and continuous learning process. The model captures short-term memory as trajectories of actions and observations, while long-term memory encompasses accumulated experiences. The interaction between these memory types and the reflective loop ensures that the agent's memory is not only a repository of past events but also a dynamic foundation for future improvement and learning. This system exemplifies how LLMs can evolve from static knowledge bases to dynamic entities capable of self-improvement through iterative reflection and adaptation. In S3 (Gao et al., 2023), the LLMs' ability to reflect is intricately tied to their simulation of human social interactions, where they continuously adjust their understanding and responses based on evolving social dynamics and cues. This reflective capacity enables them to navigate complex social environments with greater finesse. In the work of Li et al. (2024b), reflection is leveraged to refine the LLMs' approach to socio-economic predictions. By reflecting on past interactions and trends, these models can adapt their predictive algorithms, leading to more accurate responses to future social and economic shifts.

In summary, in the realm of simulating actions, LLMs stand out for their ability to integrate planning, memory, and reflection. They employ a cyclical approach where planning dictates the course of action, memory provides a knowledge base derived from past experiences, and reflection adjusts strategies based on feedback. This dynamic interplay allows LLMs to not only execute actions within varied simulations but also to continuously learn and adapt. By simulating these cognitive processes, LLMs demonstrate an advanced capacity for autonomous decision-making, which is increasingly indistinguishable from human-like behavior in complexity and adaptability.

In summary, how the large language model agents generate actions are inspired by the mechanism of humans, including planning, memory, and reflection, with similar and simplified designs. These designs are independent of the specific large language models but also significantly influence the simulation performance.

### Evaluation of LLM agents

**Realness validation with real human data.** The basic evaluation protocol for LLM-based agents is to compare the simulation's output with existing real-world data. The evaluation can be conducted at two levels: micro-level and macro-level. Specifically, micro-level evaluation refers to evaluating the ability to simulate the individual agent's behavior or actions as realistically as possible. For example, in S<sup>3</sup> (Gao et al., 2023), the authors test the performance of the LLM agents in predicting the individual agent's next state, given the current state and the environment context. On the other hand, since the agent-based simulation always pays more attention to the emerged phenomenon of the population, macro-level evaluation is of great significance, which aims to evaluate whether the simulated process has the same pattern, regularity, etc., as the real-world data. In S<sup>3</sup> (Gao et al., 2023), one of the main goals is to accurately predict the dynamics of information, opinion, and attitude based on the collected real-world social media data. In economics simulation by Li et al. (2024b), the simulated economic system is evaluated on whether those most representative macroeconomic regularities, such as Okun's law (Plosser and Schwert, 1979), etc. Furthermore, the generated behaviors' rationality can also be evaluated, such as logical consistency, adherence to established common sense, or following the given rule in the simulation environment. In addition, we can assess the simulated agent's performance against established benchmarks or standardized tasks relevant to its domain. For example, whether the agent can reach human-level evaluation scores in a web-browsing or game environment (Chang et al., 2024).

**Provide explanations for simulated behaviors.** One of the main advantages of the large language model-based agent against the traditional rule-based or neural network-based agent is its strong ability to engage in interactive conversation and textual reasoning. Therefore, to evaluate whether the agent has understood the simulation rules well, accurately perceived the environment, made a choice rationally, etc., we can directly obtain explanations from the large language model-based agent. We can evaluate whether the agent-based simulation is good by analyzing the explanations and comparing them with the human data or a well-established theory or model. For example, in economic simulation (Li et al., 2024b), the authors query the large language model agent about the reason for economic decision-making, which well explains the simulated actions and behaviors.

**Ethics evaluation.** Besides the simulation accuracy or explainability of the large language model-empowered agent-based

simulation, the ethics issue is also of great importance. The first one is bias and fairness, and it is essential to assess the simulation for biases in language, culture, gender, race, or other sensitive attributes to evaluate whether the generated content perpetuates or mitigates societal biases. Another concern is harmful output detection since the output of the generative artificial intelligence is hard to control compared with traditional approaches. Thus, the practitioners of the large language model agent-based simulation should scrutinize the simulation's output for potentially harmful or inappropriate content, including hate speech, misinformation, or offensive material.

In summary, the evaluation of the large language model for agent-based modeling and simulation mainly involves accuracy, explainability, and ethics. For accuracy, the evaluation can be conducted at both the individual level and population level, based on collected real ground-truth data; for explainability, the agent should be able to provide reliable reasons for their generated actions; for the ethics evaluation, the agent-based modeling and simulation system built with large language model agents may be faced with bigger concerns compared with traditional agent-based modeling methods, since LLM-empowered agents are much more intelligent.

### Recent advances in LLM agent-based modeling and simulation

In the following, we elaborate on the recent advances in using large language models for agent-based modeling and simulation in social, physical, cyber, and hybrid domains. The typical applications in the first three domains are illustrated in Fig. 3, and the details are shown in Table 1. We also illustrate the ratio of different domains and what to simulate in Fig. 4. From the perspective of technical design, the statistics are as follows: about 50% of the papers have considered planning when generating actions, 50% of the papers have used the reflection strategy, 80% have conducted real-world evaluation, and about 40% have considered ethical evaluation. Note that almost all the papers have designed a memory mechanism.

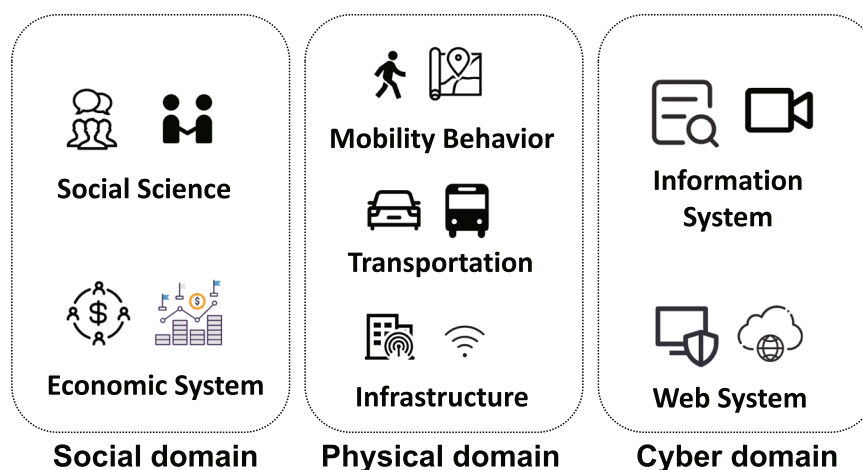
**Social domain I: social sciences.** This section discusses the application of LLM agent-based modeling and simulation in social sciences. Specifically, the existing works examine and explore LLM agents' effectiveness in replicating human behaviors and interactions and their role in validating social theories. They focus on how LLM agents can serve as tools for understanding complex social dynamics, enhancing collaborative problem-

solving, etc., offering insights into both individual and collective social behaviors, as illustrated in Fig. 5.

*Simulation of social network dynamics.* The part discusses whether LLM Agents, due to their human-like behavior, can be used to recreate and validate established social laws and patterns. This involves an analysis of how closely these agents can mimic human behavior and whether their actions can be quantified to validate or challenge existing theories in social science.

S3 (Gao et al., 2023) utilizes LLM-empowered agents to simulate individual and collective behaviors within the social network. This system effectively replicates human behaviors, including emotion, attitude, and interaction behaviors. It leverages real-world social network data to initialize the simulation environment, where information influences users' emotions and subsequent behaviors. The study particularly focuses on scenarios of gender discrimination and nuclear energy, demonstrating the ability of LLMs to simulate complex social dynamics. The results underscore LLM's ability to capture real-world social phenomena. Specifically, for the individual-level evaluation, the authors mainly focus on the prediction problem, i.e., whether the LLM agent can predict the next label (emotion, attitude, interaction). For example, whether the LLM agent can accurately predict whether the user will have a positive attitude toward one specific event. For the population-level evaluation, the authors test whether the simulated results with large language model agents have the same trends as the ground-truth data, including the propagation speed/range, attitude dynamic, etc. Williams et al. (2023) study whether LLM agents can accurately reproduce the trend of epidemic spread. The results show that the LLM agent-based simulation system can replicate complex phenomena observed in the real world, such as multi-peak patterns.

Xu et al. (2023b) examine LLMs' capabilities in simulating individual and collective behaviors in a rule-based *Werewolf Game* environment. It reveals that LLMs can effectively engage in strategic social interactions, generating behaviors such as trust and confrontation, thus offering insights into their potential for social simulations. Acerbi and Stubbersfield (2023) demonstrate that the information transmitted by large language models mirrors the biases inherent in human social communication. Specifically, LLM exhibits preferences for stereotype-consistent, negative, socially oriented, and threat-related content, reflecting biases in its training data. The observation underscores that LLMs are not neutral agents; instead, they echo and potentially amplify existing human biases, shaping the information they generate and transmit. Zhang et al. (2023c) studied the impact of collaboration strategies on the performance of LLM agents. Specifically, three



**Fig. 3** Illustration of LLM agent-based modeling and simulation in different domains.

**Table 1 A list of representative works of agent-based modeling and simulation with large language models.**

Domain	Environment	Advance	What to simulate
Social	Virtual	Schwitzgebel et al. (2024)	Conversation and interaction
Social	Virtual	Xu et al. (2023b)	Werewolf game
Social	Virtual	Acerbi and Stubbersfield (2023)	Information Propagation
Social	Virtual	Zhang et al. (2023c)	Collaboration Mechanism
Social	Virtual	Suzuki and Arita (2024)	Cooperation and defection
Social	Virtual	de Zarzà et al. (2023)	Social interaction
Social	Real	Mukobi et al. (2023)	Welfare diplomacy game
Social	Real	S3 (Gao et al., 2023)	Online social network
Social	Virtual	SimReddit (Park et al., 2022)	Online forum
Social	Real	Cai et al. (2024)	Social Media Language
Social	Real	Papachristou and Yuan (2024)	Social Network Dynamics
Social	Real	COLA (Lan et al., 2024)	Cooperative task solving
Social	Virtual	MAD (Liang et al., 2023)	Cooperative task solving
Social	Virtual	CHATDEV (Qian et al., 2024)	Cooperative task solving
Social	Virtual	MetaGPT (Hong et al., 2024)	Cooperative task solving
Social	Virtual	ChatEval (Chan et al., 2024)	Cooperative task solving
Social	Virtual	CAMEL (Li et al., 2023d)	Cooperative task solving
Social	Virtual	AgentVerse (Chen et al., 2024)	Cooperative task solving
Social	Virtual	SPP (Wang et al., 2023d)	Cooperative task solving
Social	Virtual	CoELA (Zhang et al., 2024b)	Cooperative task solving
Social	Real	Agent Hospital (Li et al., 2024a)	Cooperative task solving
Social	Virtual	Humanoid Agents (Wang et al., 2023c)	Individual social behavior
Social	Real	SocioDojo (Cheng and Chin, 2024)	Individual social behavior
Social	Virtual	Liu et al. (2024a)	Individual social behavior
Social	Virtual	Argyle et al. (2023)	Individual social behavior
Social	Virtual	Hämäläinen et al. (2023)	Individual social behavior
Social	Virtual	Singh et al. (2023)	Individual social behavior
Social	Virtual	Binz and Schulz (2023)	Individual social behavior
Social	Virtual	Elyoseph et al. (2023)	Individual social behavior
Social	Virtual	Li et al. (2022)	Individual social behavior
Social	Virtual	Xie and Zou (2024)	Individual social behavior
Social	Virtual	Yoon et al. (2024)	Individual social behavior
Social	Virtual	Horton (2023)	Economic system: individual behavior
Social	Virtual	Chen et al. (2023e)	Economic system: individual behavior
Social	Virtual	Geerling et al. (2023)	Economic system: individual behavior
Social	Real	Xie et al. (2023)	Economic system: market behavior
Social	Real	Faria-e Castro and Leibovici (2023)	Economic system: market behavior
Social	Real	Bybee (2023)	Economic system: market behavior
Social	Virtual	Phelps and Russell (2023)	Economic system: game theory
Social	Virtual	Akata et al. (2023)	Economic system: game theory
Social	Virtual	Guo et al. (2023)	Economic system: game theory
Social	Virtual	Zhao et al. (2023b)	Economic system: consumption market
Social	Virtual	Han et al. (2023)	Economic system: consumption market
Social	Virtual	Zhao et al. Nascimento et al. (2023)	Economic system: consumption market
Social	Virtual	Chen et al. (2023c)	Economic system: auction market
Physical	Real	Shah et al. (2023a)	Navigation behavior
Physical	Real	NLMap (Chen et al., 2023b)	Navigation behavior
Physical	Real	Zou et al. (2023)	Wireless network users
Physical	Real	Cui et al. (2024)	Vehicle drivers
Physical	Virtual	GITM (Zhu et al., 2023c)	Tool-usage simulation in sandbox game
Cyber	Real	WebAgent (Gur et al., 2024)	Human behaviors in Web
Cyber	Real	Mind2Web (Deng et al., 2024)	Human behaviors in Web
Cyber	Real	Zhou et al. (2024a)	Human behaviors in Web
Cyber	Real	Park et al. (2023)	Human behaviors in Web
Cyber	Virtual	RecAgent (Wang et al., 2023b)	Interaction with recommender system
Cyber	Virtual	Agent4Rec (Zhang et al., 2024a)	Interaction with recommender system
Hybrid	Virtual	Williams et al. (2023)	Epidemic spreading
Hybrid	Virtual	Generative agents (Park et al., 2023)	Sandbox social life
Hybrid	Real	WarAgent (Hua et al., 2023)	War simulation
Hybrid	Real	Li et al. (2024b)	Economic system: macroeconomics
Hybrid	Real	UGI (Xu et al., 2023a)	Human behaviors in real-world city

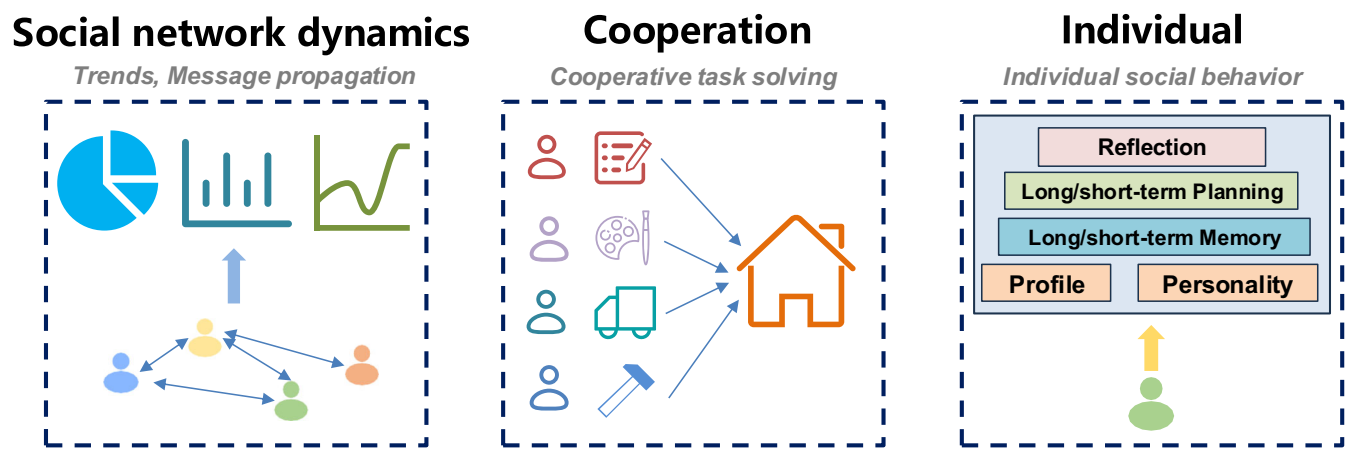
agents with distinct personalities (easy-going or overconfident) formed four different societies, employing eight collaboration strategies over three rounds to solve mathematical problems. It means that strategies initiating a debate show better results than

those relying solely on memory reflection. That is, it highlights LLM agents' capability to exhibit human-like social phenomena of conformity and the Wisdom of Crowds effect, where collective intelligence tends to surpass individual capabilities. Kim and Lee





**Fig. 4** Illustration of the ratio of different domains and simulation objectives of the recent works of large language model agent-based modeling and simulation.



**Fig. 5 Taxonomy of LLM-based modeling and simulation in social sciences.** The representative works include (Gao et al., 2023), ChatDev (Qian et al., 2024), and Humanoid agents (Wang et al., 2023c).

(2023) assessed the boundaries and effectiveness of LLMs in modeling personal actions and societal dynamics, shedding light on their applicability for believable social simulations. Suzuki and Arita (2024) and de Zarzà et al. (2023) constructed simulation systems with multiple agents, employing LLM as a generator of social strategy variations to simulate changes in cooperation/selfish strategies among agents in social cooperation and

variations in social network structures, among other factors. Park et al. (2022) investigated LLM agents' capacity to simulate online behaviors within forums. It demonstrates how LLMs can predict user interactions and responses by generating scenarios based on specific forum rules and descriptions. This simulation assists in refining forum regulations, highlighting the potential of LLMs in understanding and shaping digital social environments.

Cai et al. (2024) employed a multi-agent simulation framework using to study language evolution in regulated social media. It features LLM-driven supervisory and participant agents, simulating communication under strict regulations. The framework evaluates scenarios from abstract to real-world, demonstrating LLMs' ability to adapt language strategies, improving evasion of supervision and information accuracy. Papachristou and Yuan (2024) examined the behavior of LLM agents in forming social networks, comparing their dynamics to human social behaviors. The study highlights key principles such as preferential attachment, triadic closure, homophily, community structure, and the small-world phenomenon, revealing that LLMs' network formation decisions are influenced more by triadic closure and homophily than preferential attachment.

*Simulation of cooperation.* Some other works pay attention to the human collaboration replicated by LLM agents. Specifically, they focus on how these agents, assigned distinct roles and functions, can mimic the cooperative behaviors observed in real human societies. The mechanisms and cooperative frameworks designed for these agents can enable them to work together efficiently toward achieving goals.

COLA (Lan et al., 2024) proposed to organize LLM agents to discuss and finally decide the stance on social media text, with three role-played agents: analyzer, debater, and summarizer. The analyzers dissect texts from linguistic, domain-specific, and social media perspectives; the debaters propose logical links between text features and stances; finally, the summarizer considers all these discussions and determines the text's stance. The framework achieves SOTA performance on stance detection tasks. MAD (Liang et al., 2023) proposed to use LLM agents to engage in reasoning-intensive question answering through structured debates. LLMs adopt the roles of opposing debaters, each arguing for a different perspective on the solution's correctness. MAD enforces a "tit for tat" debate dynamic, wherein each agent must argue against the other's viewpoint, leading to a more comprehensive exploration of potential solutions. A judge agent then evaluates these arguments to arrive at a final conclusion. This work fosters divergent thinking and deep contemplation, addressing the degeneration-of-thought issue common in self-reflection methods. CHATDEV (Qian et al., 2024) is a virtual software development company where LLM Agents collaborate to develop computer software, with different roles for agents including CEO, CTO, designers, and programmers. The cooperation process encompasses designing, coding, testing, and documenting, with agents engaging in role-specific tasks like brainstorming, code development, GUI designing, and documentation. MetaGPT (Hong et al., 2024) also introduced a novel framework for collaborative software development with LLM agents, simulating a software company. The roles the agents play, including Product Manager, Architect, Project Manager, Engineer, and QA Engineer, that follows the standardized operating procedures. Each role contributes sequentially, from requirement analysis and system design to task distribution, coding, and quality assurance, showcasing LLMs' potential in efficiently mimicking human cooperative behaviors and workflows in complex software development. ChatEval (Chan et al., 2024) present a multi-agent framework for text quality evaluation, employing LLMs as diverse role-playing agents, in which key roles include the public, critics, journalists, philosophers, and scientists, each contributing unique perspectives. The agents engage in sequential debates, with access to all communication history. Finally, a judge gives a final decision. It results in more accurate and human-aligned evaluations compared to single-agent methods. CAMEL (Li et al., 2023d) introduces a cooperative role-playing framework with communicative agents,

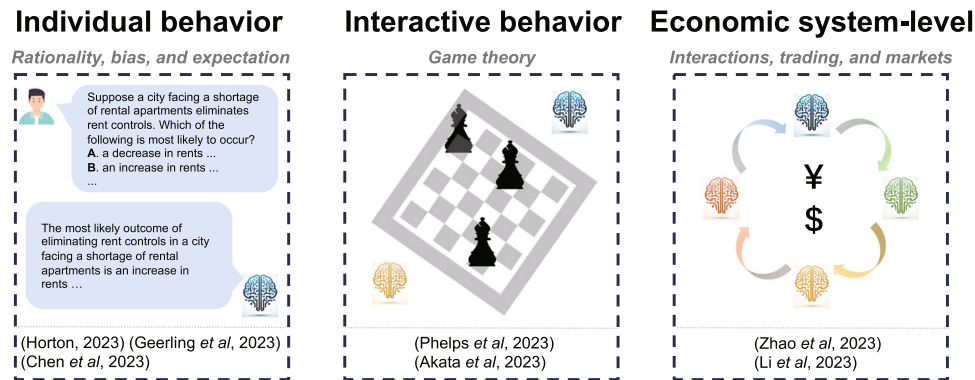
focusing on tool development. It involves roles like Task Detailing Assistant, Commander, and Executor. Specifically, Task Detailing Assistant specifies tasks in detail, Commander provides step-by-step instructions based on these specifics, and Executor carries out these instructions. Li et al. (2024a) introduced Agent Hospital, a simulation of the entire process of treating illness using LLM agents, and proposed the MedAgent-Zero method, demonstrating improved treatment performance and real-world applicability.

The above efforts involve designing specific types of agents, their roles, and the collaboration framework for certain tasks. The limitation lies in their lack of versatility, as the design of the agents is not flexible or adaptable. To address it, some work focuses on adaptively performing tasks with automated generated LLM agents and cooperation framework. AgentVerse (Chen et al., 2024) simulated human group problem-solving focusing on adaptively generating LLM agents for diverse tasks. It involves four stages: (1) Expert Recruitment, where agent composition is determined and adjusted; (2) Collaborative Decision-Making, where agents plan problem-solving strategies; (3) Action Execution, where agents implement these strategies; (4) Evaluation, assessing progress, and guiding improvements. That is, it can effectively enhance agents' capabilities across various tasks, from coding to embodied AI, demonstrating their versatility in collaborative problem-solving. Wang et al. (2023d) introduce solo performance prompting (SPP) to emulate human-like cognitive synergy, which transforms a single LLM into a multi-persona agent, enhancing problem-solving in tasks requiring complex reasoning and domain knowledge. For tasks like trivia creative writing and logic grid puzzles, SPP significantly outperforms standard methods, showcasing its effectiveness in collaborative problem-solving. CoELA (Zhang et al., 2024b) integrates LLMs' critical capabilities, including natural language processing, reasoning, and communication, into a novel cognitive-inspired modular framework. The authors evaluate CoELA in various embodied environments like C-WAH and TDW-MAT, demonstrating its proficiency in perceiving, reasoning, communicating, and planning. The results show that CoELA surpasses traditional planning methods and exhibits effective cooperation and communication behaviors.

In conclusion, simulating collaborative behaviors among LLM agents in various frameworks has shown their potential in emulating human cooperative behaviors to tackle a wide range of problem-solving tasks.

*Simulation of individual social behavior.* In the simulation of social dynamics and cooperative problem-solving, LLM agents show a strong ability to replicate human behavior. However, achieving a closer approximation to real human responses from the individual perspective is also of great significance. In this section, we discuss how the recent works approach the problem how to better simulate the individual human behavior in a social context with LLM agents, enhancing their decision-making processes, interaction patterns, and emotional responses.

Humanoid agents (Wang et al., 2023c) propose a novel approach to enhancing the realism of LLM agent simulations. By incorporating elements of human cognitive processing (System 1 (Daniel, 2017)), such as basic needs, emotions, and relational closeness, Humanoid Agents are designed to behave more like humans. For each agent, the authors maintain an internal state (stored in files) including human needs and emotions. The human needs and emotions are generated by agents with role-playing prompts, and are updated according to the context and environment changes. These dynamic elements allow agents to adapt their activities and interactions based on their internal states, thereby bridging the gap between simulated and real human behavior. The platform also facilitates immersive



**Fig. 6** Taxonomy of LLM-based modeling and simulation in economic systems.

visualization and analysis of these behaviors, advancing the field of social simulation and cooperative problem-solving. This approach demonstrates a significant leap in individual agent design, moving closer to replicating the complexities of human decision-making and interaction patterns. SocioDojo (Cheng and Chin, 2024) is a lifelong learning environment using real-world data for training agents in societal analysis and decision-making. It introduces an innovative Analyst–Assistant–Actuator framework and Hypothesis–Proof prompting, resulting in notable improvements in the time series forecasting task. Liu et al. (2024a) present a novel approach to optimizing LLM agents by refining agents’ decision-making processes, interaction patterns, and emotional responses through a three-stage alignment learning framework, Stable Alignment. This framework, which efficiently teaches social alignment to LLMs, is based on simulated social interactions, detailed feedback, and progressive refinement of responses by autonomous social agents. Xie and Zou (2024) developed a human-like planning framework for LLM agents, focusing on the multi-phase travel planning problem. By simulating human planning patterns, the framework enables LLM agents to generate coherent outlines, integrate information collection, and provide essential details.

Moreover, some studies use LLM agents to simulate human responses in social science research. Argyle et al. (2023) use LLM agents as proxies for specific human populations to generate responses in social science research. The authors show that, conditioned on socio-demographic profiles, LLM agents can generate outputs similar to human counterparts. Hämäläinen et al. (2023) construct LLM agents to simulate real participants to fill in open-ended questionnaires and analyze the similarity between the response and real data. The results show that synthetic responses generated by large language models cannot be easily distinguished from human data. Yoon et al. (2024) introduced a protocol to use LLM agents to simulate human behavior in conversational recommender systems. By assessing baseline simulators, the study identifies deviations between language models and human behavior, providing insights on improving model accuracy through better model selection and prompting strategies. In short, these works indicate that LLM agents can be useful in social science experiments to simulate human responses with much lower costs.

Some researchers have also studied LLM agents’ ability to simulate human behavior in social psychological experiments. Specifically, these works (Binz and Schulz, 2023; Singh et al., 2023) use psychological tests to simulate the human response to test the cognitive ability, emotional intelligence (Elyoseph et al., 2023), and psychological well-being (Li et al., 2022) of LLMs, demonstrating that LLM agents have human-like intelligence to a certain degree.

**Social domain II: economic system.** This section discusses another important field in the social domain, the economic system. Currently, LLM-driven economic simulations can be categorized into three types based on the number of agents involved: individual behavior, interactive behavior, and economic system-level simulations. For individual behavior simulations, the primary goal of related research is to simulate the human-like economic decision-making capabilities of LLMs (Bauer et al., 2023; Chen et al., 2023e; Geerling et al., 2023; Horton, 2023) or their understanding of economic phenomena (Bybee, 2023; Faria-e Castro and Leibovici, 2023; Xie et al., 2023). This provides an empirical foundation for the latter two types of economic simulations and is currently a more extensively researched area. In interactive behavior simulations, the focus is mainly on game theory, exploring widely focused behaviors of LLMs during game-playing, such as cooperative and reasoning behaviors (Akata et al., 2023; Guo S et al., 2024; Guo et al., 2023; Phelps and Russell, 2023). For system-level simulations, the research primarily targets market simulations, such as consumption markets or auction markets, and investigates the rationality or optimality of LLMs’ economic behaviors within these markets (Weiss M et al., 2024; Chen et al., 2023c; Li et al., 2024b; Zhao et al., 2023b). The illustration is shown in Fig. 6.

**Individual economic behavior simulation.** Considering the human-like characteristics of LLMs, many researchers attempted to replace humans in behavioral economics experiments with LLMs to observe the rational and irrational factors in their economic decision-making. Horton (2023) replicated classic behavioral economics experiments using LLMs, including unilateral dictator games, fairness constraints (Kahneman et al., 1986), and status quo bias (Samuelson and Zeckhauser, 1988), confirming the human-like nature of LLMs in aspects such as altruism, fairness preferences, and status quo bias (Horton, 2023). Although the experiment was conducted simply by asking GPT questions and analyzing responses, this represents a preliminary attempt to explore the use of LLMs for simulating human economic behavior. Chen et al. (2023e) have employed standard frameworks, *revealed preference theory*, to simulate the rationality in the economic decisions of GPTs. Results show that GPT performs largely rationally in risk, time, social, and food preferences domains in terms of budgetary decisions. Additionally, Geerling et al. (2023) have utilized the Test of Understanding in College Economics to simulate LLMs’ comprehension of microeconomics and macroeconomics, with results indicating that LLMs outperform most students who have taken economics courses.

Another research line to test the economic capabilities of LLMs involves accurately understanding certain socio-economic phenomena, specifically by using external text information (such as news) to



predict future economic changes. Xie et al. (2023) used LLM to predict stock market movements with historical stock data and related tweets based on the perception of investor sentiment. However, the predictive performance of LLMs is worse than that of state-of-the-art methods, and in some cases, it is even inferior to traditional linear regression. Faria-e Castro and Leibovici (2023) utilized LLMs for quarterly inflation forecasts, achieving accuracy comparable to, if not surpassing, the results of the Survey of Professional Forecasters (SPF). Bybee (2023) tested LLMs on their predictions of finance and macroeconomics after reading specific sections of The Wall Street Journal, with results equivalent to those of SPF. These results suggest that LLMs possess a basic understanding of economic and financial markets but still lack sufficient and precise perception for accurate prediction, requiring more domain-specific data for additional fine-tuning.

*Interactive economic behavior simulation.* These simulations mainly focus on game theory, where there are only two or a few agents as opponents. Observing and analyzing the interactive behavior and capabilities of LLMs in various classic games is a current research hotspot. Guo (2023) studied the behavior of large language model agents in the ultimatum game and prisoner's dilemma game and found that the agents exhibit some similar patterns as humans, such as the positive correlation between offered amounts and acceptance rates in the ultimatum game. Phelps and Russell (2023) found that incorporating individual preferences into prompts can influence the level of cooperation of LLMs. Specifically, they construct LLM agents with different personalities like competitive, altruistic, self-interested, etc., via prompts. Then, they let the agents play the repeated prisoner's dilemma game with bots with fixed strategies (e.g. always cooperate, always defect, or tit-for-tat) and analyze the agents' cooperation rate. They find that competitive and self-interested LLM agents show a lower cooperation rate, while altruistic agents demonstrate a higher cooperation rate, indicating the feasibility of constructing agents with different preferences through natural language. However, LLM agents also have limitations in some capabilities, such as the inability to reasonably respond to opponents' actions, which may lead to higher cooperation preferences with betraying opponents. The understanding of LLM social behaviors is very important for subsequent developments in artificial intelligence and its impact on human social behavior. Other research (Guo S et al., 2024) measured LLMs' rationality and strategic reasoning ability using the second-price auction and the Beauty Contest game. In such games, fully rational players are assumed to choose the most beneficial choice from their point of view, which results in the Nash equilibrium. Therefore, the authors define the deviation of LLMs' behavior from Nash equilibrium as the rationality degree. Moreover, they measure the strategic reasoning ability of LLMs by the ratio of the actual payoff to the optimal payoff. Experiments show that LLMs generally demonstrate rationality to some degree while they often cannot reach the Nash equilibrium. Among them, GPT-4 shows better strategic reasoning ability and can converge to Nash equilibrium faster than other LLMs like GPT-3.5 and text-davinci. The authors claim to provide a benchmark for testing the economic capabilities of the LLM research community. Akata et al. (2023) discovered through experiments in multiple game scenarios that LLMs are skilled in games valuing their self-interest but not as adept at coordinating with others. Specifically, in the prisoner's dilemma, GPT-4 will cooperate well with a cooperative opponent but will always choose to defect after the opponent defects once. In the Battle of the Sexes, GPT-4 cannot coordinate well with the opponent's choices to obtain maximum payoff.

In addition to the observations on the cooperative behavior and reasoning abilities of LLM agents during gaming, there are

also a few studies attempting to construct strong game-playing agents. Guo et al. (2023) go beyond simple measurement and enhance LLMs' gaming abilities through prompt engineering. This work, specifically in an incomplete information game (namely Leduc Hold'em), has created agents with higher-order theory of mind that can significantly outperform traditional algorithm-based opponents without the requirement for training. Meta Fundamental AI Research Diplomacy Team (FAIR)<sup>†</sup> et al., (2022) proposed the first AI agent Cicero combining a language model and reinforcement learning to play the Diplomacy game. After competing with real humans in online games anonymously, results show that Cicero can outperform 90% of players. Even without employing LLMs, it has been demonstrated that earlier language models can approach or even surpass human capabilities in the realm of strategic gaming. Moreover, Mao et al. (2023) developed a simulation framework named *Alympics*, consisting of a sandbox playground and several agent players. The sandbox playground serves as the environment that stores and executes game settings, and agent players interact with the environment. The framework enables controlled, scalable, and reproducible simulation of game theory experiments.

The results from these simple simulation environments further validate the perception, reasoning, and planning capabilities of LLMs. In order to maximize their goals, LLMs consider their own benefits and opponents' strategies when making economic decisions. It is worth noting that these goals can be customized through prompts, such as maximizing returns or maximizing fairness.

*Economic system-level simulation.* In an economic system, agents often interact with each other, trade goods, and form a market. These agents may not be limited to individuals but can also represent entities such as companies and banks, as these are also important components of the market. Zhao et al. (2023b), through simple consumption market simulations, uncovered competitive behaviors of LLM agents in managing restaurants, which are aligned with well-known sociological and economic theories. Specifically, the dish prices tend to be consistent with each other in the two simulated restaurants. Matthew effect also emerges during the simulation, i.e., one restaurant becomes more popular and popular while another has few consumers. Moreover, restaurants imitate competitors' behaviors, and at the same time, they try to make differentiation to attract more consumers. Similarly, Han et al. (2023) studied the collusion between firms' price strategies. They simulated the product pricing process of two firms in a market environment (i.e., Bertrand duopoly game) based on LLM. The results show that in the absence of communication, prices tend to approach the Bertrand equilibrium price. However, with communication, collusion between the companies tends to bring prices closer to the monopoly price. Nascimento et al. (2023) simulated a simple online book marketplace and observed interesting phenomena such as price negotiation between sellers and buyers. Another work (Weiss M et al., 2024) attempts to have LLMs act as intermediaries in information trading markets to address the issue of information asymmetry between buyers and sellers. Specifically, when a seller presents information and quotes a price as the response to the query from a buyer, an LLM agent, acting as an intermediary, can decide whether to purchase and, if choosing not to, forget the information seen, thus protecting the seller's interests. In experiments, the information to exchange is actually the 'passage' from documents on the topic of LLMs from ArXiv. The results show that LLM can not only make rational purchasing decisions in this information market but also ensure the rationality of the overall market dynamics; for example, a higher budget can improve the quality of purchased answers (response to queries).

Chen et al. (2023c) have developed LLM agents with planning capabilities in constructed virtual auction markets to achieve higher profits given limited budgets. Experiments show that LLM has the crucial abilities to participate in the auction, including managing budgets, considering long-term returns, etc., even through only simple prompts.

**Physical domain.** For the physical domain, the applications for LLM agent-based modeling and simulation include mobility behaviors, transportation, wireless networks, etc.

*LLM agents for simulating mobility behaviors.* Understanding real-world space and time is crucial to harness LLMs for agent-based modeling and simulation in human mobility behaviors. Researchers have delved into this issue through various investigations (Gurnee and Tegmark, 2024; Manvi et al., 2024). Gurnee and Tegmark (2024) focus on probing LLMs to extract representations of real-world locations and temporal events, and the results demonstrate that these models build spatial and temporal representations in the neural layers. Manvi et al. (2024) delve into the geospatial knowledge embedded in LLMs. By fine-tuning LLMs on map-based prompts, substantial geospatial knowledge within LLMs is illustrated and shows improvements in tasks related to population density, asset wealth, and education. These investigations contribute valuable insights into the nuanced understanding of real-world space and time by LLMs, laying the groundwork for their application in agent-based simulations.

Based on their fundamental abilities, LLMs have showcased remarkable capabilities in simulation for the physical domain. For simulating the human-like navigation behaviors in the physical environment, LM-Nav (Shah et al., 2023) combines large language models with image-language alignment algorithms. Following it, LLM-Planner (Song et al., 2023) harnesses large language models to achieve few-shot planning for embodied agents. Moving into the domain of real-world planning with large language models, Chen et al. (2023b) introduce NLMap, which creates an open-vocabulary and queryable scene representation, allowing language models to gather and integrate contextual information for context-conditioned planning. Additionally, Shah et al. (2023b) study training a general goal-conditioned model to simulate human-like vision-based navigation, demonstrating the broad generalization capabilities of LLMs in complex physical environments.

*LLM agent-based modeling and simulation for transportation.* The possibility of using LLM agents for other applications in the physical domain, like transportation, has also been explored. Jin et al. (2023) design an LLM agent to simulate the driving behavior of human drivers. Specifically, the agent interacts with a simulator named CARLA, where it receives information about the state of the car and environment from the simulator and decides what to do next, such as stop, speed up, change lanes, and so on, which will be fed back to the simulator. During the decision process, the agent will consider its recent behaviors using a memory module and also take into account safety criteria as well as guidelines learned from human expert drivers. Experiments show that the agent design can significantly reduce collision rate and make the agent's behavior more human-like. Moreover, the agent manages to perform complex driving tasks such as overtaking.

*LLM agent-based modeling and simulation for wireless network.* In addition, some researchers focus on deploying LLM agents to simulate device users in the city infrastructure, such as the wireless network. Zou et al. (2023) propose a framework where multiple on-device LLM agents can interact with the environment

and exchange knowledge to solve a complex task together. Specifically, intents from humans or machines are provided to agents through wireless terminals, and the tasks are divided and planned collaboratively among multiple agents by leveraging the knowledge of different LLMs and device capabilities. On each device, the agent observes the environment and acts to execute decisions. On-device LLMs can extract semantic information from various data types and store it for future task planning. To deal with a specific task, the agent can retrieve relevant information or create lower-level tasks and send them to other agents to achieve the goal. The authors demonstrate the ability of the framework by an example of a wireless energy-saving task, where four users aim to reduce the network energy consumption while keeping the transmission rate. In the experiment, the agents gradually decrease their own power level based on previous actions of other users and manage to achieve the target after a few iterations, which shows the potential of LLM agent-based modeling and simulation in solving wireless network problems.

**Cyber domain.** Agent-based modeling and simulation cyberspace mainly involves various human behaviors such as information access, website visitation, network attack/defense, etc., in cyberspace.

WebAgent (Gur et al., 2024) is introduced as an LLM-driven agent capable of learning from its experiences to simulate human behaviors on real websites based on natural language instructions. It strategizes by breaking down instructions into manageable subparts, condenses lengthy HTML documents into relevant sections for the task at hand, and interacts with websites using Python programs derived from this information. Mind2Web (Deng et al., 2024) further used large language models (LLMs) to construct these generalist web agents. While the sheer size of raw HTML from real websites poses a challenge for LLMs, Mind2Web demonstrates that pre-filtering this data with a smaller language model substantially enhances the effectiveness and efficiency of the LLMs in generating human-like web browsing behaviors. Zhou et al. (2024a) further addressed the discrepancy between current language-guided autonomous agents, often tested in simplified synthetic environments and the complexity of real-world scenarios. The authors build a highly realistic and reproducible environment specifically tailored for language-guided agents simulating human behaviors on the web. Park et al. (2023) simulate online decision-making scenarios, exploring the challenges individuals face when lacking domain expertise while searching for and making decisions using online information. Wang et al. (2023b) proposed to build large language models to interact with recommender systems by selecting from recommendation results and providing positive or negative feedback. It serves as the testing protocol for evaluating the recommender system's performance: whether it can satisfy the agents' preferences well.

In RecAgent (Wang et al., 2023b), the researchers explore the potential of LLMs in simulating user behaviors within online environments, particularly recommender systems. By creating an LLM-based autonomous agent framework, the study investigates how these agents can simulate complex human interactions and decisions in a virtual environment. This approach enables a novel method for studying user behavior, offering insights into how users might react to different scenarios in digital platforms, thus advancing our understanding of user dynamics in virtual spaces. Zhang et al. (2024a) proposed to build generative agents for the recommender system in which the authors design LLM-empowered generative agents equipped with user profile, memory, and actions modules specifically tailored for the recommender system. The proposed agents can emulate the filter

bubble effect and discover the underlying causal relationships in recommendation tasks.

**Hybrid domain.** In some studies, simulations are conducted that simultaneously consider more than one domain, such as physical and social, and we refer to these simulations as being within a hybrid domain.

As a pioneering work, Generative Agents (Park et al., 2023) offers a compelling insight into the generation of believable individual and social behaviors. The research focuses on a central question: how can generative agents reliably produce human-like individual actions and social dynamics? It delves into an agent architecture that integrates memory (for storing past experiences), reflection (to make rational present decisions), and planning (for future actions). This architecture is critically evaluated through crowd-sourced assessments, affirming the effectiveness of the memory, reflection, and planning modules in generating rational behaviors. Notably, this approach led to complex social scenarios, such as Valentine's Day parties and mayoral elections, underscoring the agents' proficiency in simulating nuanced human interactions and societal events. This research offers a substantial contribution to social simulations, demonstrating the advanced potential of LLM agents in replicating the depth and complexity of human social behaviors.

Williams et al. (2023) conducted an epidemic simulation within a hybrid domain. In this simulation, social relationships influenced individuals' perception of the epidemic, while individuals' physical movements within spatial contexts affected their susceptibility to infection. Welfare Diplomacy (Mukobi et al., 2023) sets a benchmark, a nation-to-nation war/welfare equilibrium tabletop game designed to evaluate the collaborative capabilities of large language models.

Hua et al. (2023) proposed to use LLM agents to represent countries and simulate their decisions and consequences, based on which the historical international conflicts, including World War I, World War II, and the Warring States Period in Ancient China are selected for evaluation. In the LLM agent-based war simulations, the emergent interactions among countries help explain why the wars occur.

Li et al. (2024b) simulate a hybrid macroeconomic system and expand the scale of simulation environments from tens to hundreds. Specifically, they simulate LLM-empowered agents' work and consumption behaviors in a macroeconomic market. The proposed perception, memory, and action modules endow the agents with real-world heterogeneity, the ability to grasp market dynamics, and decision-making considering multiple economic factors, respectively. Experimental results show the emergence of more reasonable and stable macroeconomic indicators (price inflation, unemployment rate, GDP, and GDP growth rate) and regularities (Phillips curve and Okun's law) compared with traditional rule-based ABM (Gatti et al., 2011; Lengnick, 2013) and RL-based approaches (Zheng et al., 2022). Especially, only the simulation based on LLM agents can produce the correct Phillips curve, i.e., negative relationship between the unemployment rate and inflation. This advantage is owned by LLM's accurate perception of market dynamics, such as the deflation of labor markets.

Urban generative intelligence (UGI) (Xu et al., 2023a) is a platform that constructs a real-world urban environment provided by digital twins, which provide various interfaces for embodied agents to generate many behaviors, supported by a foundation model named CityGPT, which is trained on city-specific multi-source data. In this platform, multiple categories of LLM-based agents can simulate human-like behaviors, including social interactions, economic activities, mobility, street

navigation, etc., showing promising abilities in simulating city activities based on embodied agents.

### Open problems and future directions

**Efficiency of scaling up.** Many studies of LLM agents find it advantageous to simultaneously simulate multiple personas and exploit the synergy effect by allowing them to communicate and vote for the final output (Yao et al., 2024). For example, researchers find LLM-based software development can be significantly improved by simulating a virtual software company with diverse social identities, including chief officers, professional programmers, test engineers, and art designers (Qian et al., 2024). This virtual company is capable of streamlining the development of complex software solutions in the stages of designing, coding, testing, and documenting. Moreover, researchers generally find scaling up the number of simulated agents and deploying more diverse personas are beneficial in various tasks (Zhuge et al., 2023).

However, simulating societies of large-scale LLM agents is very computationally expensive. Extensive research efforts are dedicated to optimizing the memory footprint (Sheng et al., 2023) and operation subroutines (Aminabadi et al., 2022) of language models. Researchers also develop several effective model compression techniques (Zhu et al., 2023d), such as knowledge distillation and quantization. In the context of LLM agent simulation, batch prompting (Cheng et al., 2023b) is a highly relevant technique that is capable of simulating multiple agents in batches. Experiments show batch prompting can achieve up to 5× efficiency improvement in inference token and time costs. Besides, MetaGPT is proposed to improve the efficiency of multi-agent collaboration in virtual software companies Hong et al. (2024). They leverage a shared message pool and subscribe mechanism to reduce the time and token cost of generating one line of code. Despite the previous efforts of accelerating LLM agents, simulating large-scale LLM agents remains a highly challenging task, which significantly hinders LLM agent simulation from reaching its full potential. Simulating large societies of LLM agents not only can effectively improve the performance in downstream tasks but also has the potential to mimic the emergence properties of human societies and, hence, reveal the underlying mechanisms (Caldarelli et al., 2023). Therefore, it is an important open problem to achieve full-process acceleration of LLM agent simulations.

**Benchmark.** Benchmarks have significantly advanced the development of AI in the past decade. Landmark benchmarks like ImageNet (Russakovsky et al., 2015), GLUE (Wang et al., 2019), and the benchmarks in graph learning (Dwivedi et al., 2023; Hu et al., 2020) have been pivotal to the rapid innovation in the fields of computer vision, natural language processing, and graph neural networks.

Recently, there has been a surge in benchmarks that assess the capabilities of LLM-driven agents, highlighting the growing interest in this emerging area. For example, researchers Valmeekam et al. (2022) developed benchmarks to evaluate LLM's capability in planning and reasoning about change, focusing on symbolic models and structured inputs compatible with such representations. Meanwhile, AgentBench develops a multi-dimensional benchmark with eight distinct environments to assess the capabilities of LLM-driven agents in various multi-turn open-ended generation settings (Liu et al., 2024b). MAgentBench, on the other hand, designs a suite of ML tasks for benchmarking LLM-driven AI research agents, including tasks like image classification and sentiment classification (Huang et al., 2023). Researchers also propose to evaluate LLM-driven



agents with embodied tasks, using them as high-level planners in robotics setups or in textual environments, focusing on the interaction between planning and action, like ALFWorld (Shridhar et al., 2021) and ComplexWorld (Basavatia et al., 2023). On top of textual environments, online reinforcement learning approaches are developed to align LLM agents with human preferences and evaluate their performance (Carta et al., 2023).

However, the previous benchmarks mainly focus on the decision and planning capability of LLM-driven agents, the assessment of LLM-driven agent simulation is still inadequate. On the one hand, there still exist challenges in evaluating the performance of agent simulations. Previous works often examine the statistics feature of simulated behavior (Feng et al., 2020), such as the spatial and temporal distribution. Recent studies also recruit human evaluators to gather feedback on the believability of the simulation (Park et al., 2023). However, developing benchmarks for quantitative and qualitative evaluation of LLM-driven agent-based simulation remains a largely open problem and a promising future research direction. On the other hand, LLM-driven simulation might serve as a realistic environment that provides high-quality feedback to train other AI models. For example, previous studies explore the simulations of social segregation (Sert et al., 2020), competing firms (Osoba et al., 2020), competitive games (Park et al., 2019), and coordination of different stakeholders (Bone and Dragičević, 2010). Such simulations can serve as a benchmark to train and evaluate the reinforcement learning models. A recent study by Wu et al. (2023) proposes a PET framework to leverage LLM-driven agents as a supervisor of low-level trainable models, which simplifies challenging control tasks by translating task descriptions into high-level sub-tasks and then tracking the accomplishment of these sub-tasks. Additionally, more research efforts should be dedicated to the benchmarks of AI for social good (Cowls et al., 2021).

**Open platform.** Building open platforms for LLM-driven agents will play a pivotal role in this emerging research area that could substantially reduce the barriers of LLM-driven ABS and foster a vibrant community, echoing the calls for open-source software (Weber, 2004) and open science National Academies of Sciences et al. (2018). The recent advance of LLMs has led to the public release of several powerful pre-trained language models. For example, Bidirectional Encoder Representations from Transformers (BERT) has been publicly released and gained huge influence in the past few years (Devlin et al., 2019). GPT2, a predecessor to the current ChatGPT family, was released by OpenAI with limited model sizes for open-source use (Radford et al., 2019). Additionally, Meta AI recently released a collection of open foundation and fine-tuned chat models named LLaMa 2 (Touvron et al., 2023), which range in scale from 7 billion to 70 billion parameters. These open-source LLMs demonstrate powerful capabilities in various natural language tasks, which can be further adapted for specific downstream tasks with efficient fine-tuning methods such as Low-Rank Adaptation (LoRA) (Hu et al., 2021).

The recent proliferation of LLM-driven agents has also resulted in several open-source platforms. Voyager is an example open-source framework of embodied LLM-driven agents, capable of continuously acquiring diverse skills and making novel discoveries in Minecraft without human intervention (Xi et al., 2023). Researchers also develop open-source frameworks for real-world task-solving agents, such as XAgent Team (2024) that are designed as a general-purpose framework of automatic task-solving. Moreover, ModelScope-Agent (Li et al., 2023b) is

proposed as a general and customizable agent framework designed for real-world applications, which supports model training on multiple open-source LLMs and offers diversified and comprehensive APIs. On top of the textual embodied environment ALFWorld, researchers developed BUTLER framework (Shridhar et al., 2021) that can operate across text and embodied environments with three main components, i.e., brain, vision, and body. This arrangement allows BUTLER to effectively bridge the gap between abstract language understanding and practical, embodied task execution in simulated virtual environments. However, these previous works mainly focus on task-solving LLM agents, while the open platforms for LLM-driven ABS are still lacking. Such a gap can be largely attributed to the challenges of integrating LLM-driven agents with the complex environment of simulation. Urban generative intelligence (UGI) (Xu et al., 2023a) is a recently proposed open platform that integrates embodied agents with the digital twins of cities, offering the opportunity to evaluate urban problems with large-scale urban agent simulations and solve them with multi-disciplinary approaches. Despite this early attempt at urban system simulation, the development of an open platform for LLM-driven ABS is an emerging area that calls for more research attention.

**Robustness of LLM-driven agent-based simulation.** The robustness problems of LLM agent simulation can be classified into two main scenarios, adversarial attack and out-of-distribution generalization, which fundamentally stem from the robustness issues of the underlying language models (Wang et al., 2023a). The current methodologies to address out-of-distribution generalization problems primarily resort to classic machine learning techniques (Shen et al., 2021), such as unsupervised representation learning, supervised model learning, and optimization methods. As for adversarial attacks, various defense techniques have been proposed in recent studies. For example, researchers propose to certify LLM safety with an erase-and-check filter that detects adversarial prompts (Kumar et al., 2023). Besides moving target defense, Chen et al. (2023a) aim to select safe answers from the responses generated by different LLMs to enhance the LLM system's robustness against jailbreaking attacks. Moreover, extensive benchmarks of adversarial prompts are formulated to evaluate LLM (Zhu et al., 2023b).

As for the LLM agents, they often have tool-use capability (Qin et al., 2023) and engage in human interactive scenarios, such as the conflict simulation actor that helps users learn conflict resolve through rehearsal (Shaikh et al., 2024), which makes the robustness of LLM agents have far-reaching consequences. Furthermore, in the context of multi-agent simulation, adversarial attacks might propagate among agents (Tian et al., 2023). More importantly, recent works show the simulations of multiple LLM agents show human-like collective behaviors (Aher et al., 2023; Zhou et al., 2024b), such as social conformity and homophily, which could be exploited by adversaries as weaknesses in the societies of LLM agents. Improving the robustness of LLM agent simulation at both the individual and collective levels is an open problem.

The stability of LLM agents can also be regarded as one kind of robustness. Even if the LLM agents are fed the same prompts, the agent may generate odd responses due to the limitation of large language models, especially for smaller LLMs. This leads to a concern about the reproducibility of large language model-empowered agent-based modeling and simulation. Three potential solutions exist based on the requirements of agent-based modeling and simulation and the characteristics of large language models. The first solution is to develop specialized large language

models tailored for simulation, improving environment consistency. The second solution may be a combination of large and smaller LLMs, reaching an acceptable trade-off between cost and robustness. The third promising future direction could be a better agent mechanism, with more powerful reflection, memory, etc.

**Ethical risks in LLM agents.** The advances of LLM unleash the unprecedented capability of human-like text generation and reasoning, raising concerns about potential ethical risks of misuse, such as jailbreaking (Zhuo et al., 2023). For example, recent studies highlight the risks of generating malicious network payloads that could jeopardize cyber security at scale (Charan et al., 2023), and emphasize the concerns of accuracy, recency, coherence, and transparency of LLM agents in medical practice (Thirunavukarasu et al., 2023). To gauge LLM agents' susceptibility to social bias and stereotype, researchers use semantic illusions and cognitive reflection tests (Hagendorff et al., 2023), typically administered to human subjects, to quantify LLM's tendency to produce intuitive yet erroneous responses. They find early models from the GPT family have an increasing tendency to generate intuitive errors as their size increases, while ChatGPT-3.5 and 4 have a pattern shift that radically eliminates these errors and achieves superhuman accuracy. They speculate the pattern shift is driven by the employment of reinforcement learning from human feedback, a sophisticated technique only deployed in ChatGPT-3.5 and later models. These findings highlight the importance of embedding human preferences into the language models, instead of solely relying on web corpus. In the context of LLM-driven agent simulations, researchers find when certain personas are assigned to ChatGPT it will generate output with 6× toxicity, engaging in discriminatory stereotypes, harmful conversation, and offensive language (Deshpande et al., 2023). Besides, a recent work by Acerbi and Stubbersfield (2023) shows LLM agent exhibits human-like biases that prefer gender-stereotype-consistent, negative, and biologically counter-intuitive content. More importantly, such biases could be further amplified in the transmission chain in multi-agent settings. The experimental results from previous studies emphasize the importance of ethical considerations in LLM-driven agent-based simulations, especially against the backdrop of the rapid proliferation of LLM agents in various domains.

Extensive efforts have been made to mitigate the potential ethical risks of LLM agents. A primary focus is to fundamentally align language models with human values (Yao et al., 2023a; Yi et al., 2023). A recent survey classifies the alignment goals into three distinct levels, i.e., human instructions, human preferences, and human values. Besides, Moral Foundation theory is invoked to benchmark mainstream language models' alignment with the foundational ethical values of care, fairness, loyalty, authority, and sanctity (Yi et al., 2023). Researchers also find LLM agents are susceptible to flattened caricatures when specific personas are assigned to them (Cheng et al., 2023a). The CoMPoS framework is proposed to evaluate the multidimensionality of simulated LLM agents and provide a measure for caricature in LLM agent simulations. They find even the agents driven by the latest GPT-4 in the simulation of political and marginalized demographic groups. Finally, to fundamentally address the potential ethical risks, many scholars advocate enhancing the interpretability of LLM agents, questioning the falsifiability of any moral principles learned by black box LLM agents (Vijayaraghavan and Badea, 2024). Therefore, they propose to benchmark and continuously improve LLM agents' interpretability (Zhao et al., 2024).

## Conclusion

Agent-based modeling and simulation is one of the most important methods to model complex systems in various domains. The recent advances in large language models have

reshaped the paradigm of agent-based modeling and simulation, providing a new perspective for constructing intelligent human-like agents rather than those driven by simple rules or limited-intelligence neural models. In this paper, we take the first step to provide a survey of the agent-based modeling and simulation with large language models. We systematically analyze why the LLM agents are required for agent-based modeling and simulation and how to address the critical challenges. Afterward, we extensively summarize the existing works in four domains: cyber, physical, social, and hybrid, carefully describing how to design the simulation environment, how to construct the large language model-empowered agents, and what to observe and achieve based on agent-based simulation. Lastly, given the unresolved limitations of existing works and this new and fast-growing area, we discuss the open problems and point out the important research directions, which we hope can inspire future research.

## Data availability

All data generated or analyzed during this study are included in this manuscript.

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## References

- Acerbi A, Stubbersfield JM (2023) Large language models show human-like content biases in transmission chain experiments. *Proc Natl Acad Sci USA* 120:e2313790120
- Aher GV, Arriaga RI, Kalai AT (2023) Using large language models to simulate multiple humans and replicate human subject studies. In: *International Conference on Machine Learning (PMLR)*. pp 337–371
- Akata E et al. (2023) Playing repeated games with large language models. *arXiv preprint arXiv:2305.16867*
- Alluhaybi B, Alrahhhal MS, Alzhirani A, Thayanathan V (2019) A survey: agent-based software technology under the eyes of cyber security, security controls, attacks and challenges *Int J Adv Comput Sci Appl* 10:211–230
- Aminabadi RY et al. (2022) DeepSpeed-inference: enabling efficient inference of transformer models at unprecedented scale. In: *SC22: international conference for high performance computing, networking, storage and analysis*. IEEE, pp 1–15. <https://ieeexplore.ieee.org/abstract/document/10046087>
- An L (2012) Modeling human decisions in coupled human and natural systems: review of agent-based models. *Ecol Model* 229:25–36
- Antonini G, Bierlaire M, Weber M (2006) Discrete choice models of pedestrian walking behavior. *Transp Res Part B: Methodol* 40:667–687
- Argyle LP et al. (2023) Out of one, many: using language models to simulate human samples. *Political Anal* 31:337–351
- Arora D, Singh HG et al. (2023) Have LLMs advanced enough? A challenging problem solving benchmark for large language models. *The 2023 Conference on Empirical Methods in Natural Language Processing*. <https://openreview.net/forum?id=YHWWXIESeS8>
- Arsanjani JJ, Helbich M, de Noronha Vaz E (2013) Spatiotemporal simulation of urban growth patterns using agent-based modeling: the case of Tehran. *Cities* 32:33–42
- Arthur WB (1991) Designing economic agents that act like human agents: a behavioral approach to bounded rationality. *Am Econ Rev* 81:353–359
- Bakhtin A, Brown N, Dinan E, Farina G, Flaherty C, Fried D, Goff A, Gray J, Hu H, Jacob APMeta Fundamental AI Research Diplomacy Team (FAIR)† (2022) Human-level play in the game of diplomacy by combining language models with strategic reasoning *Science* 378:1067–1074
- Banisch S, Lima R, Araújo T (2012) Agent based models and opinion dynamics as Markov chains. *Soc Netw* 34:549–561
- Barbosa J, Leirão P (2011) Simulation of multi-agent manufacturing systems using agent-based modelling platforms. In: *Proceedings of the 2011 9th IEEE international conference on industrial informatics*. IEEE, pp 477–482
- Barnes S, Golden B, Price S (2013) Applications of agent-based modeling and simulation to healthcare operations management. In: *Price CC & Gendreau M (eds) Handbook of healthcare operations management: methods and applications*. Springer, pp. 45–74. <https://www.springer.com/series/6161>
- Barros JX (2004) Urban growth in Latin American cities-exploring urban dynamics through agent-based simulation. University of London, University College London, UK

- Basavatia S, Ratnakar S, Murugesan K (2023) Complexworld: a large language model-based interactive fiction learning environment for text-based reinforcement learning agents. *International Joint Conference on Artificial Intelligence 2023 Workshop on Knowledge-Based Compositional Generalization*
- Batty M (2001) Agent-based pedestrian modeling. *Environ plan B: Plan Des* 28:321–326
- Bauer K, Liebich L, Hinz O, Kosfeld M (2023) Decoding GPT's Hidden 'Rationality' of Cooperation. *SAFE Working Paper No. 401*, <https://doi.org/10.2139/ssrn.4576036>
- Beheshti R, Jalalpour M, Glass TA (2017) Comparing methods of targeting obesity interventions in populations: an agent-based simulation. *SSM-Popul Health* 3:211–218
- Bellegarda JR (2004) Statistical language model adaptation: review and perspectives. *Speech Commun* 42:93–108
- Beltran RS, Testa JW, Burns JM (2017) An agent-based bioenergetics model for predicting impacts of environmental change on a top marine predator, the Weddell seal. *Ecol Model* 351:36–50
- Binz M, Schulz E (2023) Using cognitive psychology to understand GPT-3. *Proc Natl Acad Sci USA* 120:e2218523120
- Bohmann JD, Calantone RJ, Zhao M (2010) The effects of market network heterogeneity on innovation diffusion: an agent-based modeling approach. *J Product Innov Manag* 27:741–760
- Boiko DA, MacKnight R, Gomes G (2023) Emergent autonomous scientific research capabilities of large language models. *arXiv preprint arXiv:2304.05332*
- Bone C, Dragičević S (2010) Simulation and validation of a reinforcement learning agent-based model for multi-stakeholder forest management. *Comput Environ Urban Syst* 34:162–174
- Bran AM, Cox S, White AD, Schwaller P (2023) Chemcrow: augmenting large-language models with chemistry tools. *arXiv preprint arXiv:2304.05376*
- Brown T et al. (2020) Language models are few-shot learners. *Adv Neural Inf Process Syst* 33:1877–1901
- Brown DG, Robinson DT (2006) Effects of heterogeneity in residential preferences on an agent-based model of urban sprawl. *Ecol Soc* 11
- Bybee L (2023) Surveying generative AI's economic expectations. *arXiv preprint arXiv:2305.02823*
- Cabrera E, Taboada M, Iglesias ML, Epelde F, Luque E (2011) Optimization of healthcare emergency departments by agent-based simulation. *Procedia Comput Sci* 4:1880–1889
- Cai J et al. (2024) Language evolution for evading social media regulation via llm-based multi-agent simulation. *IEEE WCCI*, <https://arxiv.org/abs/2405.02858>
- Caldarelli G et al. (2023) The role of complexity for digital twins of cities. *Nat Comput Sci* 3:374–381
- Carta T et al. (2023) Grounding large language models in interactive environments with online reinforcement learning. *International Conference on Machine Learning*. PMLR, pp 3676–3713
- Chan C-M et al. (2024) ChatEval: towards better LLM-based evaluators through multi-agent debate. *The Twelfth International Conference on Learning Representations*. <https://openreview.net/forum?id=FQepisCUWu>
- Chang Y et al. (2024) A survey on evaluation of large language models. *ACM Trans Intell Syst Technol* 15:1–45
- Charan P, Chunduri H, Anand PM, Shukla SK (2023) From text to mitre techniques: exploring the malicious use of large language models for generating cyber attack payloads. *arXiv preprint arXiv:2305.15336*
- Chen L (2012) Agent-based modeling in urban and architectural research: a brief literature review. *Front Archit Res* 1:166–177
- Chen B et al. (2023b) Open-vocabulary queryable scene representations for real world planning. In *2023 IEEE International Conference on Robotics and Automation (ICRA)*. IEEE, pp 11509–11522
- Chen B, Paliwal A, Yan Q (2023a) Jailbreaker in jail: moving target defense for large language models. In: *Proceedings of the 10th ACM Workshop on Moving Target Defense*. pp 29–32
- Chen J, Yuan S, Ye R, Majumder BP, Richardson K (2023c) Put your money where your mouth is: evaluating strategic planning and execution of LLM agents in an auction arena. *arXiv preprint arXiv:2310.05746*
- Chen W et al. (2024) Agentverse: Facilitating multi-agent collaboration and exploring emergent behaviors in agents. *The Twelfth International Conference on Learning Representations*. <https://openreview.net/forum?id=EHg5GDnyq1>
- Chen Y, Liu TX, Shan Y, Zhong S (2023e) The emergence of economic rationality of GPT. In: *Proceedings of the National Academy of Sciences*. Vol 120. National Acad Sciences, p e2316205120
- Cheng J, Chin P (2024) SocioDojo: Building Lifelong Analytical Agents with Real-world Text and Time Series. *The Twelfth International Conference on Learning Representations*. <https://openreview.net/forum?id=s9z0HzWJp>
- Cheng M, Piccardi T, Yang D (2023a) Compost: characterizing and evaluating caricature in LLM simulations. In: *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*. Association for Computational Linguistics, pp 10853–10875
- Cheng Z, Kasai J, Yu T (2023b) Batch prompting: efficient inference with large language model APIs. In: *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*. Association for Computational Linguistics, Singapore, pp 792–810, <https://doi.org/10.18653/v1/2023.emnlp-industry.74>
- Chowdhery A et al. (2023) Palm: scaling language modeling with pathways. *J Mach Learn Res* 24:1–113
- Cipi E, Cico B (2011) Simulation of an agent based system behavior in a dynamic and unpredicted environment. *Simulation* 1:172–176
- Conte R, Paolucci M (2014) On agent-based modeling and computational social science. *Front Psychol* 5:668
- Cowls J, Tsamados A, Taddeo M, Floridi L (2021) A definition, benchmark and database of AI for social good initiatives. *Nat Mach Intell* 3:111–115
- Cui C, Ma Y, Cao X, Ye W, Wang Z (2024) Drive as you speak: enabling human-like interaction with large language models in autonomous vehicles. In: *Proceedings of the IEEE/CVF Winter Conference on Applications of Computer Vision*, pp 902–909
- de Souza F, Verbas O, Auld J (2019) Mesoscopic traffic flow model for agent-based simulation. *Procedia Comput Sci* 151:858–863
- de Zarza I, de Curtò J, Roig G, Manzoni P, Calafate CT (2023) Emergent cooperation and strategy adaptation in multi-agent systems: an extended coevolutionary theory with LLMs. *Electronics* 12:2722
- DeepMind G (2023) Introducing Gemini: our largest and most capable AI model. <https://blog.google/technology/ai/google-gemini-ai>. Accessed 7 Dec 2023
- Deguchi H (2011) Economics as an agent-based complex system: toward agent-based social systems sciences. *Springer Science & Business Media*
- Deng X et al. (2024) Mind2web: towards a generalist agent for the web. *Adv Neural Inf Process Syst*, 36
- Deshpande A, Murahari V, Rajpurohit T, Kalyan A, Narasimhan K (2023) Toxicity in chatgpt: analyzing persona-assigned language models. *Findings of the Association for Computational Linguistics: EMNLP 2023*, Association for Computational Linguistics, pp 1236–1270. <https://doi.org/10.18653/v1/2023.findings-emnlp.88>
- Devlin J, Chang M-W, Lee K, Toutanova K (2019) Bert: pre-training of deep bidirectional transformers for language understanding. In: *Proceedings of naacL-HLT Vol 1*. pp 2
- Dong Q et al. (2022) A survey for in-context learning. *arXiv preprint arXiv:2301.00234* (2022)
- Dubois Y et al. (2024) AlpacaFarm: a simulation framework for methods that learn from human feedback. *Adv Neural Inf Process Syst*, 36
- Dwivedi VP et al. (2023) Benchmarking graph neural networks. *J Mach Learn Res* 24:1–48
- Elliott E, Kiel LD (2002) Exploring cooperation and competition using agent-based modeling. *Proc Natl Acad Sci USA* 99:7193–7194
- El-Sayed AM, Scarborough P, Seemann L, Galea S (2012) Social network analysis and agent-based modeling in social epidemiology. *Epidemiol Perspect Innov* 9:1–9
- Elsenbroich C, Gilbert N, Elsenbroich C, Gilbert N (2014) Agent-based modelling. *Modelling Norms*, pp 65–84
- Elyoseph Z, Hadar-Shoval D, Asraf K, Lvovsky M (2023) Chatgpt outperforms humans in emotional awareness evaluations. *Front Psychol* 14:1199058
- Faria-e Castro M, Leibovici F (2023) Artificial intelligence and inflation forecasts. *Technical Report*, <https://research.stlouisfed.org/wp/more/2023-015>
- Feng L, Li B, Podobnik B, Preis T, Stanley HE (2012) Linking agent-based models and stochastic models of financial markets. *Proc Natl Acad Sci USA* 109:8388–8393
- Feng J et al. (2020) Learning to simulate human mobility. In: *Proceedings of the 26th ACM SIGKDD international conference on knowledge discovery & data mining*. pp 3426–3433
- Franceschelli G, Musolesi M (2023) On the creativity of large language models. *arXiv preprint arXiv:2304.00008*
- Fu D et al. (2024) Drive like a human: rethinking autonomous driving with large language models. In: *Proceedings of the IEEE/CVF Winter Conference on Applications of Computer Vision*. pp 910–919
- Gao C et al. (2023) S3: social-network simulation system with large language model-empowered agents. *arXiv preprint arXiv:2307.14984*
- Gatti DD, Desiderio S, Gaffeo E, Cirillo P, Gallegati M (2011) Macroeconomics from the Bottom-up, Vol 1. *Springer Science & Business Media*
- Gaube V, Remesch A (2013) Impact of urban planning on household's residential decisions: an agent-based simulation model for Vienna. *Environ Model Softw* 45:92–103
- Geerling W, Mateer GD, Wooten J, Damodaran N (2023) Chatgpt has aced the test of understanding in college economics: now what? *Am Econ*. 68. <https://doi.org/10.1177/05694345231169654>
- Gilbert N (2004a) Agent-based social simulation: dealing with complexity. *Complex Syst Netw Excell* 9:1–14
- Gilbert N, Terna P (2000) How to build and use agent-based models in social science. *Mind Soc* 1:57–72
- Gilbert N (2007b) Computational social science: agent-based social simulation. In: *Phan D & Amblard F (eds) Agent-based modelling and simulation*. *Bardwell, Oxford*, pp 115–134



- Gilbert N, Troitzsch K (2005) Simulation for the social scientist. McGraw-Hill Education, UK
- Guo F (2023) GPT agents in game theory experiments. arXiv preprint arXiv:2305.05516
- Guo J et al. (2023) Suspicion-agent: Playing imperfect information games with theory of mind aware GPT-4. arXiv preprint arXiv:2309.17277
- Guo S et al. (2024) Large language models as rational players in competitive economics games. In: Proceedings of the 12th international conference on learning representations. <https://openreview.net/forum?id=NMPLBbjYFq>
- Gur I et al. (2024) A real-world webagent with planning, long context understanding, and program synthesis. The Twelfth International Conference on Learning Representations. <https://openreview.net/forum?id=9JQtrumvg8>
- Gurnee W, Tegmark M (2024) Language models represent space and time. The Twelfth International Conference on Learning Representations. <https://openreview.net/forum?id=jE8xbmvFin>
- Guyot P, Honiden S (2006) Agent-based participatory simulations: merging multi-agent systems and role-playing games. J Artif Soc Soc Simul 9
- Hagendorff T, Fabi S, Kosinski M (2023) Human-like intuitive behavior and reasoning biases emerged in large language models but disappeared in ChatGPT. Nat Comput Sci, 3:833–838
- Hämäläinen P, Tavast M, Kunnari A (2023) Evaluating large language models in generating synthetic HCI research data: a case study. In: Proceedings of the 2023 CHI Conference on Human Factors in Computing Systems. ACM, pp 1–19
- Hamill L, Gilbert N (2015) Agent-based modelling in economics. John Wiley & Sons
- Han X, Wu Z, Xiao C (2023) “Guinea pig trials” utilizing GPT: a novel smart agent-based modeling approach for studying firm competition and collusion. arXiv preprint arXiv:2308.10974
- Hauser MD, Chomsky N, Fitch WT (2002) The faculty of language: what is it, who has it, and how did it evolve? science 298:1569–1579
- Heckbert S, Baynes T, Reeson A (2010) Agent-based modeling in ecological economics. Ann N Y Acad Sci USA 1185:39–53
- Helbing D, Molnar P (1995) Social force model for pedestrian dynamics. Phys Rev E 51:4282
- Helbing D (2012) Social self-organization: agent-based simulations and experiments to study emergent social behavior. Springer
- Hernández-Orallo J, Martínez-Plumed F, Schmid U, Siebers M, Dowe DL (2016) Computer models solving intelligence test problems: progress and implications. Artif Intell 230:74–107
- Hong S et al. (2024) MetaGPT: meta programming for multi-agent collaborative framework. The Twelfth International Conference on Learning Representations. <https://openreview.net/forum?id=VtmBAGCN7o>
- Horton JJ (2023) Large language models as simulated economic agents: what can we learn from homo silicus? Technical Report, National Bureau of Economic Research
- Hoshen D, Werman M (2017) IQ of neural networks. arXiv preprint arXiv:1710.01692
- Hu W et al. (2020) Open graph benchmark: datasets for machine learning on graphs. Adv Neural Inf Process Syst 33:22118–22133
- Hu EJ et al. (2022) Lora: low-rank adaptation of large language models. International Conference on Learning Representations. <https://openreview.net/forum?id=nZeVKeeFY9>
- Hua W et al. (2023) War and peace (waragent): Large language model-based multi-agent simulation of world wars. arXiv preprint arXiv:2311.17227
- Huang Q, Vora J, Liang P, Leskovec J (2023) Benchmarking large language models as AI research agents. arXiv preprint arXiv:2310.03302
- Jang J et al. (2023) Personalized soups: personalized large language model alignment via post-hoc parameter merging. arXiv preprint arXiv:2310.11564
- Jiang LY et al. (2023) Health system-scale language models are all-purpose prediction engines. Nature 619:357–362
- Jin Y et al. (2023) Surrealdriver: designing generative driver agent simulation framework in urban contexts based on large language model. arXiv preprint arXiv:2309.13193
- Jinjin S et al. (2023) CGMI: configurable general multi-agent interaction framework. arXiv preprint arXiv:2308.12503
- Kahneman D (2017) Thinking, fast and slow[J]. Farrar, Straus and Giroux, 2011
- Kahneman D, Knetsch JL, Thaler R (1986) Fairness as a constraint on profit seeking: entitlements in the market. Am Econ Rev 76.4:728–741
- Kavak H, Padilla JJ, Lynch CJ, Diallo SY (2018) Big data, agents, and machine learning: towards a data-driven agent-based modeling approach. In: Proceedings of the annual simulation symposium. pp 1–12
- Kim D, Yun T-S, Moon I-C, Bae JW (2021) Automatic calibration of dynamic and heterogeneous parameters in agent-based models. Autonomous Agents Multi-Agent Syst 35:46
- Kim J, Lee B (2023) AI-augmented surveys: leveraging large language models for opinion prediction in nationally representative surveys. arXiv preprint arXiv:2305.09620
- Kountouriotis V, Thomopoulos SC, Papelis Y (2014) An agent-based crowd behaviour model for real time crowd behaviour simulation. Pattern Recognit Lett 44:30–38
- Kovač G, Portelas R, Dominey PF, Oudeyer P-Y (2023) The social AI school: Insights from developmental psychology towards artificial socio-cultural agents. arXiv preprint arXiv:2307.07871
- Kumar A, Agarwal C, Srinivas S, Feizi S, Lakkaraju H (2023) Certifying llm safety against adversarial prompting. arXiv preprint arXiv:2309.02705
- Lan X, Gao C, Jin D, Li Y (2024) Stance detection with collaborative role-infused llm-based agents. In: Proceedings of the international AAAI conference on web and social media, AAAI, Vol 18. pp 891–903
- Lengnick M (2013) Agent-based macroeconomics: a baseline model. J Econ Behav Organ 86:102–120
- Leombruni R, Richiardi M (2005) Why are economists sceptical about agent-based simulations? Physica A 355:103–109
- Li K, Liang H, Kou G, Dong Y (2020) Opinion dynamics model based on the cognitive dissonance: An agent-based simulation. Inf Fusion 56:1–14
- Li B et al. (2023a) Seed-bench: benchmarking multimodal LLMs with generative comprehension. arXiv preprint arXiv:2307.16125
- Li C et al. (2023b) Modelscope-agent: building your customizable agent system with open-source large language models. In: Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing: System Demonstrations. Association for Computational Linguistics, Singapore, pp 566–578 <https://aclanthology.org/2023.emnlp-demo.51>
- Li C et al. (2023c) Quantifying the impact of large language models on collective opinion dynamics. arXiv preprint arXiv:2308.03313
- Li G, Hammoud HAAK, Itani H, Khizbullin D, Ghanem B (2023d) Camel: Communicative agents for “mind” exploration of large language model society. Adv Neural Inf Process Syst 36:51991–52008
- Li J et al. (2024a) Agent hospital: a simulacrum of hospital with evolvable medical agents. arXiv preprint arXiv:2405.02957
- Li N, Gao C, Li M, Li Y, Liao Q (2024b) Econagent: large language model-empowered agents for simulating macroeconomic activities. In: ACL
- Li S, Yang J, Zhao K (2023e) Are you in a masquerade? exploring the behavior and impact of large language model driven social bots in online social networks. arXiv preprint arXiv:2307.10337
- Li X, Li Y, Liu L, Bing L, Joty S (2022) Is GPT-3 a psychopath? evaluating large language models from a psychological perspective. arXiv preprint arXiv:2212.10529
- Liang T et al. (2023) Encouraging divergent thinking in large language models through multi-agent debate. arXiv preprint arXiv:2305.19118
- Lin L-J (1992) Self-improving reactive agents based on reinforcement learning, planning and teaching. Mach Learn 8:293–321
- Lin J et al. (2023) Agentsims: an open-source sandbox for large language model evaluation. arXiv preprint arXiv:2308.04026
- Lippe M et al. (2019) Using agent-based modelling to simulate social-ecological systems across scales. GeoInformatica 23:269–298
- Liu R et al. (2024a) Training socially aligned language models in simulated human society. The Twelfth International Conference on Learning Representations. <https://openreview.net/forum?id=NddKiWtdUm>
- Liu X et al. (2024b) Agentbench: evaluating LLMs as agents. The Twelfth International Conference on Learning Representations. <https://openreview.net/forum?id=zAdUB0aCTQ>
- Liu Y et al. (2019) How well do machines perform on IQ tests: a comparison study on a large-scale dataset. In: IJCAI. pp 6110–6116
- Lopez PA et al. (2018) Microscopic traffic simulation using sumo. In: 2018 21st international conference on intelligent transportation systems (ITSC). IEEE, pp 2575–2582
- Lu J et al. (2023) Self: language-driven self-evolution for large language model. arXiv preprint arXiv:2310.00533
- Luo L et al. (2008) Agent-based human behavior modeling for crowd simulation. Comput Animat Virtual Worlds 19:271–281
- Ma Y, Zhenjiang S, Kawakami M (2013) Agent-based simulation of residential promoting policy effects on downtown revitalization. J Artif Soc Soc Simul 16:2
- Macal CM, North MJ (2005) Tutorial on agent-based modeling and simulation. In: Proceedings of the Winter Simulation Conference. IEEE, 14pp
- Macy MW, Willer R (2002) From factors to actors: computational sociology and agent-based modeling. Annu Rev Sociol 28:143–166
- Madey G, Gao Y, Freeh V, Tynan R, Hoffman C (2003) Agent-based modeling and simulation of collaborative social networks. In: Proceedings Americas Conference on Information Systems (AMCIS) pp 1836–1842

- Maggi E, Vallino E (2016) Understanding urban mobility and the impact of public policies: the role of the agent-based models. *Res Transp Econ* 55:50–59
- Mańdziuk J, Zychowski A (2019) Deepiq: a human-inspired AI system for solving IQ test problems. In: 2019 International Joint Conference on Neural Networks (IJCNN). IEEE, pp 1–8
- Manvi R et al. (2024) Geollm: extracting geospatial knowledge from large language models. The Twelfth International Conference on Learning Representations. <https://openreview.net/forum?id=TqL2xBwXP3>
- Mao S et al. (2023) Alympics: language agents meet game theory. arXiv preprint arXiv:2311.03220
- Mastio M, Zargayouna M, Scemama G, Rana O (2018) Distributed agent-based traffic simulations. *IEEE Intell Transp Syst Mag* 10:145–156
- McLane AJ, Semeniuk C, McDermid GJ, Marceau DJ (2011) The role of agent-based models in wildlife ecology and management. *Ecol Model* 222:1544–1556
- Melis G, Dyer C, Blunsom P (2017) On the state of the art of evaluation in neural language models. arXiv preprint arXiv:1707.05589
- Mueller M, Pyka A (2016) Economic behaviour and agent-based modelling. In: Frantz R, Chen S-H, Dopfer K, Heukelom F, Mousavi S, (eds) Routledge handbook of behavioral economics. Routledge, pp 405–415
- Mukobi G et al. (2023) Welfare diplomacy: benchmarking language model cooperation. arXiv preprint arXiv:2310.08901
- Nascimento N, Alencar P, Cowan D (2023) Self-adaptive large language model (LLM)-based multiagent systems. 2023 IEEE International Conference on Autonomic Computing and Self-Organizing Systems Companion (ACSOS-C), IEEE, pp 104–109
- National Academies of Sciences E Medicine et al. (2018) Open science by design: realizing a vision for 21st century research
- OpenAI (2022) Introducing ChatGPT. <https://openai.com/blog/chatgpt>. Accessed 1 Dec 2023
- Osoba OA, Vardavas R, Grana J, Zutshi R, Jaycocks A (2020) Policy-focused agent-based modeling using RL behavioral models. arXiv preprint arXiv:2006.05048
- Papachristou M, Yuan Y (2024) Network formation and dynamics among multi-LLMs. arXiv preprint arXiv:2402.10659
- Park YJ, Cho YS, Kim SB (2019) Multi-agent reinforcement learning with approximate model learning for competitive games. *PLoS ONE* 14:e0222215
- Park J, Min B, Ma X, Kim J (2023) Choicemates: supporting unfamiliar online decision-making with multi-agent conversational interactions. arXiv preprint arXiv:2310.01331
- Park JS et al. (2022) Social simulacra: Creating populated prototypes for social computing systems. In: Proceedings of the 35th annual ACM symposium on user interface software and technology. ACM, pp 1–18
- Park JS et al. (2023) Generative agents: interactive simulacra of human behavior. In: Proceedings of the 36th annual ACM symposium on user interface software and technology. ACM, pp 1–22
- Parv L, Deaky B, Nasulea MD, Oancea G (2019) Agent-based simulation of value flow in an industrial production process. *Processes* 7:82
- Pereira A, Duarte P, Reis LP (2004) Agent-based simulation of ecological models. In: Proceedings 5th Workshop on Agent-Based Simulation
- Perez L, Dragicevic S (2009) An agent-based approach for modeling dynamics of contagious disease spread. *Int J Health Geogr* 8:1–17
- Pertoldi C, Topping C (2004) Impact assessment predicted by means of genetic agent-based modeling. *Crit Rev Toxicol* 34:487–498
- Phelps S, Russell YI (2023) Investigating emergent goal-like behaviour in large language models using experimental economics. arXiv preprint arXiv:2305.07970
- Platas-López A, Guerra-Hernández A, Quiroz-Castellanos M, Cruz-Ramirez N (2023) A survey on agent-based modelling assisted by machine learning. *Expert Syst* e13325. <https://doi.org/10.1111/exsy.13325>
- Plosser CI, Schwert GW (1979) Potential GNP: its measurement and significance: a dissenting opinion. In: Carnegie-Rochester conference series on public policy, Elsevier, Vol 10, pp 179–186
- Puranam P, Stieglitz N, Osman M, Pillutla MM (2015) Modelling bounded rationality in organizations: progress and prospects. *Acad Manag Ann* 9:337–392
- Qian C et al. (2024) Communicative agents for software development. In: Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Vol 1: Long Papers) Association for Computational Linguistics, Bangkok, Thailand, pp 15174–15186. <https://aclanthology.org/2024.acl-long.810>
- Qin Y et al. (2023) Tool learning with foundation models. arXiv preprint arXiv:2304.08354
- Radford A et al. (2019) Language models are unsupervised multitask learners. *OpenAI Blog* 1:9
- Rolón M, Martínez E (2012) Agent-based modeling and simulation of an automotive manufacturing execution system. *Comput Ind* 63:53–78
- Rouchier J (2017) Agent-based simulation as a useful tool for the study of markets. In: *Simulating social complexity: a handbook*. pp 671–704
- Russakovsky O et al (2015) Imagenet large scale visual recognition challenge. *Int J Comput Vis* 115:211–252
- Samanidou E, Zschischang E, Stauffer D, Lux T (2007) Agent-based models of financial markets. *Rep Prog Phys* 70:409
- Samuelson W, Zeckhauser R (1988) Status quo bias in decision making. *J Risk Uncertain* 1:7–59
- Schick T et al. (2024) Toolformer: language models can teach themselves to use tools. *Adv Neural Inf Process Syst* 36:68539–68551
- Schieritz N, Grobler A (2003) Emergent structures in supply chains—a study integrating agent-based and system dynamics modeling. In: Proceedings of the 36th Annual Hawaii International Conference on System Sciences. IEEE, 9
- Schwitzgebel E, Schwitzgebel D, Strasser A (2024) Creating a large language model of a philosopher. *Mind Lang* 39:237–259
- Sert E, Bar-Yam Y, Morales AJ (2020) Segregation dynamics with reinforcement learning and agent based modeling. *Sci Rep* 10:11771
- Shah D, Osiński B, Levine S et al. (2023a) Lm-nav: robotic navigation with large pre-trained models of language, vision, and action. In: Conference on robot learning. PMLR, pp 492–504
- Shah D, Sridhar A, Bhorkar A, Hirose N, Levine S (2023b) Gnm: a general navigation model to drive any robot. In: 2023 IEEE International Conference on Robotics and Automation (ICRA). IEEE, pp 7226–7233
- Shaikh O, Chai V, Gelfand MJ, Yang D, Bernstein MS (2024) Rehearsal: simulating conflict to teach conflict resolution. In: Proceedings of the CHI Conference on Human Factors in Computing Systems. pp 1–20
- Shanahan M, McDonell K, Reynolds L (2023) Role play with large language models. *Nature* 623:493–498
- Shen Z et al. (2021) Towards out-of-distribution generalization: a survey. arXiv preprint arXiv:2108.13624
- Sheng Y et al. (2023) High-throughput generative inference of large language models with a single gpu. International Conference on Machine Learning, PMLR, pp 31094–31116
- Shinn N, Cassano F, Gopinath A, Narasimhan KR, Yao S (2023) Reflexion: language agents with verbal reinforcement learning. In: 37th conference on Neural Information Processing Systems. <https://doi.org/10.48550/arXiv.2303.11366>
- Shridhar M et al. (2021) Alfworl: aligning text and embodied environments for interactive learning. International Conference on Learning Representations. <https://openreview.net/forum?id=0IOX0YcCdTn>
- Silva PC et al. (2020) Covid-abs: an agent-based model of COVID-19 epidemic to simulate health and economic effects of social distancing interventions. *Chaos Solitons Fractals* 139:110088
- Silverman BG, Hanrahan N, Bharathy G, Gordon K, Johnson D (2015) A systems approach to healthcare: agent-based modeling, community mental health, and population well-being. *Artif Intell Med* 63:61–71
- Simon HA (1997) Models of bounded rationality: empirically grounded economic reason, Vol 3. MIT Press
- Singh M et al. (2023) Mind meets machine: unravelling GPT-4's cognitive psychology. *BenchCouncil Trans Benchmarks, Stand Eval* 3:100139
- Singhal K et al. (2023) Large language models encode clinical knowledge. *Nature* 620:172–180
- Song CH et al. (2023) LLM-planner: few-shot grounded planning for embodied agents with large language models. In: Proceedings of the IEEE/CVF international conference on computer vision. pp 2998–3009
- Sun H, Zhuang Y, Kong L, Dai B, Zhang C (2024) Adaplaner: adaptive planning from feedback with language models. *Adv Neural Inf Process Syst* 36:58202–58245
- Surowiecki J (2005) The wisdom of crowds. Anchor
- Suzuki R, Arita T (2024) An evolutionary model of personality traits related to cooperative behavior using a large language model. *Sci Rep* 14:5989
- Taori R et al. (2023) Stanford alpaca: an instruction-following llama model. [https://github.com/tatsu-lab/stanford\\_alpaca](https://github.com/tatsu-lab/stanford_alpaca)
- Team A (2022) Autogpt: the heart of the open-source agent ecosystem. <https://github.com/Significant-Gravitas/AutoGPT>. Accessed 1 Oct 2023
- Team X (2024) Xagent: an autonomous agent for complex task solving | XAgent (xagent.net)
- Terna P et al. (1998) Simulation tools for social scientists: building agent based models with swarm. *J Artif Soc Soc Simul* 1:1–12
- Thirunavukarasu AJ et al. (2023) Large language models in medicine. *Nat Med* 29:1930–1940
- Tian Y, Yang X, Zhang J, Dong Y, Su H (2023) Evil geniuses: delving into the safety of LLM-based agents. arXiv preprint arXiv:2311.11855
- Tomasello M (2010) Origins of human communication. MIT Press
- Touvron H et al. (2023) Llama: open and efficient foundation language models. arXiv preprint arXiv:2302.13971
- Valmeekam K, Olmo A, Sreedharan S, Kambhampati S (2022) Large language models still can't plan (a benchmark for LLMs on planning and reasoning about change). arXiv preprint arXiv:2206.10498

- Van Dinther C (2008) Agent-based simulation for research in economics. In: Handbook on information technology in finance. Springer, pp 421–442
- Vijayaraghavan A, Badea C (2024) Minimum levels of interpretability for artificial moral agents. AI and Ethics, Springer, pp 1–17
- Wall F (2016) Agent-based modeling in managerial science: an illustrative survey and study. *Rev Manag Sci* 10:135–193
- Wang A et al. (2019) Glue: a multi-task benchmark and analysis platform for natural language understanding. 7th International Conference on Learning Representations, ICLR 2019
- Wang G et al. (2024a) Voyager: an open-ended embodied agent with large language models. *Transactions on Machine Learning Research*, pp 2835–8856 <https://openreview.net/forum?id=ehfRiF0R3a>
- Wang J et al. (2023a) On the robustness of ChatGPT: an adversarial and out-of-distribution perspective. *arXiv preprint arXiv:2302.12095*
- Wang L et al. (2023b) Recagent: a novel simulation paradigm for recommender systems. *arXiv preprint arXiv:2306.02552*
- Wang L et al. (2024b) A survey on large language model based autonomous agents. *Front Comput Sci* 18:186345
- Wang L, Ahn K, Kim C, Ha C (2018) Agent-based models in financial market studies. *J Phys Conf Ser* 1039, 012022
- Wang Z, Chiu YY, Chiu YC (2023c) Humanoid agents: platform for simulating human-like generative agents. *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing: System Demonstrations*, pp 167–176
- Wang Z et al. (2023d) Unleashing cognitive synergy in large language models: A task-solving agent through multi-persona self-collaboration. *arXiv preprint arXiv:2307.05300*
- Weber S (2004) The success of open source. Harvard University Press
- Wei J et al. (2022) Chain-of-thought prompting elicits reasoning in large language models. *Adv Neural Inf Process Syst* 35:24824–24837
- Weiss M et al. (2024) Rethinking the buyer's inspection paradox in information markets with language agents. In: *Proceedings of the 12th international conference on learning representations*. <https://openreview.net/forum?id=6werMQy1uz>
- Widener MJ, Metcalf SS, Bar-Yam Y (2013) Agent-based modeling of policies to improve urban food access for low-income populations. *Appl Geogr* 40:1–10
- Williams R, Hosseinichimeh N, Majumdar A, Ghaffarzadegan N (2023) Epidemic modeling with generative agents. *arXiv preprint arXiv:2307.04986*
- Wolfram S (1984) Cellular automata as models of complexity. *Nature* 311:419–424
- Wooldridge M, Jennings NR (1995) Intelligent agents: theory and practice. *Knowl Eng Rev* 10:115–152
- Wu Y et al. (2023) Plan, eliminate, and track—language models are good teachers for embodied agents. *arXiv preprint arXiv:2305.02412*
- Xi Z et al. (2023) The rise and potential of large language model based agents: A survey. *arXiv preprint arXiv:2309.07864*
- Xie C, Zou D (2024) A human-like reasoning framework for multi-phases planning task with large language models. *arXiv preprint arXiv:2405.18208*
- Xie Q, Han W, Lai Y, Peng M, Huang J (2023) The Wall Street Neophyte: a zero-shot analysis of chatgpt over multimodal stock movement prediction challenges. *arXiv preprint arXiv:2304.05351*
- Xu F, Zhang J, Gao C, Feng J, Li Y (2023a) Urban generative intelligence (UGI): a foundational platform for embodied agent and future city. *arXiv:2312.11813*
- Xu Y et al. (2023b) Exploring large language models for communication games: an empirical study on werewolf. *arXiv preprint arXiv:2309.04658*
- Yao S et al. (2024) Tree of thoughts: deliberate problem solving with large language models. *Adv Neural Inf Process Syst* 36:11809–11822
- Yao J, Yi X, Wang X, Wang J, Xie X (2023a) From instructions to intrinsic human values—a survey of alignment goals for big models. *arXiv preprint arXiv:2308.12014*
- Yi X, Yao J, Wang X, Xie X (2023) Unpacking the ethical value alignment in big models. *arXiv preprint arXiv:2310.17551*
- Yoheinakajima (2023) Babyagi. <https://github.com/yoheinakajima/babyagi>. Accessed 1 Oct 2023
- Yoon S-E, He Z, Echterhoff JM, McAuley J (2024) Evaluating large language models as generative user simulators for conversational recommendation. In: *Proceedings of the 2024 conference of the north american chapter of the association for computational linguistics: human language technologies (Vol 1: Long Papers)*, Association for Computational Linguistics, pp 1490–1504. <https://doi.org/10.18653/v1/2024.naacl-long.83>
- Zeng A et al. (2023) Glm-130b: an open bilingual pre-trained model. In: *Proceedings of the 11th international conference on learning representations*
- Zhang B, DeAngelis DL (2020) An overview of agent-based models in plant biology and ecology. *Ann Bot* 126:539–557
- Zhang A et al. (2024a) On generative agents in recommendation. In: *Proceedings of the 47th international ACM SIGIR conference on research and development in Information Retrieval*, pp 1807–1817
- Zhang H et al. (2024b) Building cooperative embodied agents modularly with large language models. The Twelfth International Conference on Learning Representations. <https://openreview.net/forum?id=EnXJfQy0K>
- Zhang J, Xu X, Deng S (2023c) Exploring collaboration mechanisms for LLM agents: a social psychology view. *arXiv preprint arXiv:2310.02124*
- Zhang T et al. (2024c) Benchmarking large language models for news summarization. *Trans Assoc Comput Linguist* 12:39–57
- Zhao H et al. (2024) Explainability for large language models: a survey. *ACM Trans Intell Syst Technol* 15:1–38
- Zhao Q et al. (2023b) Competeai: understanding the competition behaviors in large language model-based agents. *arXiv preprint arXiv:2310.17512*
- Zhao WX et al. (2023c) A survey of large language models. *arXiv preprint arXiv:2303.18223*
- Zheng S, Trott A, Srinivasa S, Parkes DC, Socher R (2022) The AI economist: Taxation policy design via two-level deep multiagent reinforcement learning. *Sci Adv* 8:eabk2607
- Zhou S et al. (2024a) WebArena: A realistic Web Environment for Building Autonomous Agents. The Twelfth International Conference on Learning Representations. <https://openreview.net/forum?id=oKn9c6ytLx>
- Zhou X et al. (2024b) Sotopia: interactive evaluation for social intelligence in language agents. The Twelfth International Conference on Learning Representations. <https://openreview.net/forum?id=mM7VurbA4r>
- Zhu D, Chen J, Shen X, Li X, Elhoseiny M (2024) Minigpt-4: enhancing vision-language understanding with advanced large language models. The Twelfth International Conference on Learning Representations. <https://openreview.net/forum?id=1tZbq88f27>
- Zhu K et al. (2023b) Promptbench: towards evaluating the robustness of large language models on adversarial prompts. *arXiv preprint arXiv:2306.04528*
- Zhu X et al. (2023c) Ghost in the minecraft: generally capable agents for open-world environments via large language models with text-based knowledge and memory. *arXiv preprint arXiv:2305.17144*
- Zhu X, Li J, Liu Y, Ma C, Wang W (2023d) A survey on model compression for large language models. *arXiv preprint arXiv:2308.07633*
- Zhuge M et al. (2023) Mindstorms in natural language-based societies of mind. *arXiv preprint arXiv:2305.17066*
- Zhuo TY, Huang Y, Chen C, Xing Z (2023) Exploring ai ethics of ChatGPT: a diagnostic analysis. *arXiv preprint arXiv:2301.12867*
- Zou H, Zhao Q, Bariah L, Bennis M, Debbah M (2023) Wireless multi-agent generative AI: from connected intelligence to collective intelligence. *arXiv preprint arXiv:2307.02757*

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## Author contributions

C. Gao contributed to the structure of this survey paper, searching and organizing all relevant related papers, as well as all the content throughout the whole paper. X. Lan partly contributed to the content relevant to the social domain; N. Li and Z. Zhou partly contributed to the content relevant to the economic domain; Y. Yuan and J. Ding partly contributed to the content relevant to agent-based modeling and the physical domain. F. Xu partly contributed to the section on perspectives of this research direction. Y. Li contributed to the whole structure, motivation, and taxonomy. All authors contributed to the writing of this manuscript.

## Competing interests

The authors declare no competing interests.

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## Informed consent

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