A Survey of Large Language Models and LLM-Based Agents in Social Simulation and Computational Social Science

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Abstract

The interdisciplinary field of social simulation and computational social science has been significantly advanced by the integration of large language models (LLMs) and LLM-based agents. This survey paper explores their transformative role in simulating and analyzing social behaviors within virtual environments. LLMs, with their sophisticated natural language processing capabilities, have enhanced the realism and complexity of simulations by integrating with agent-based modeling frameworks, thereby providing nuanced insights into social dynamics. The application of LLMs spans virtual persona creation, gaming environments, and conversational AI, showcasing their versatility in modeling diverse social scenarios. Additionally, the incorporation of Theory of Mind and moral frameworks into LLM-based agents has enriched their social intelligence, enabling them to navigate complex interactions and ethical dilemmas. Despite these advancements, challenges such as computational complexity, resource constraints, and ethical considerations persist, necessitating ongoing research to address these issues. Future directions include the enhancement of simulation techniques, integration with multimodal and interdisciplinary approaches, and the expansion of applications and evaluation metrics. These developments promise to further elevate the capabilities of LLM-based simulations, offering new dimensions for understanding and analyzing the complexities of human social interactions. As research evolves, LLMs are poised to play a pivotal role in advancing the field of computational social science.

1 Introduction

1.1 Emergence and Importance of LLMs

The advent of large language models (LLMs) has profoundly transformed artificial intelligence, particularly in simulating complex human systems [1]. Their ability to integrate user preferences and environmental factors enhances the realism of social simulations, allowing for the modeling of diverse human behaviors across demographics, which is crucial for social science experiments and public opinion surveys [2, 3]. LLMs' asynchronous capabilities facilitate parallel processing and real-time tool use, overcoming the limitations of traditional synchronous AI systems and enabling dynamic simulations [4].

As LLMs evolve, their role in analyzing complex social behaviors becomes increasingly vital, especially in e-commerce contexts where they autonomously engage in actions like browsing and purchasing. This evolution enhances multi-agent systems and provides insights into social phenomena, such as herd behavior [5, 6, 7, 8]. By offering a robust framework for understanding interactions within virtual environments, LLMs contribute to the development of socially intelligent AI agents, thereby enriching simulations in computational social science.

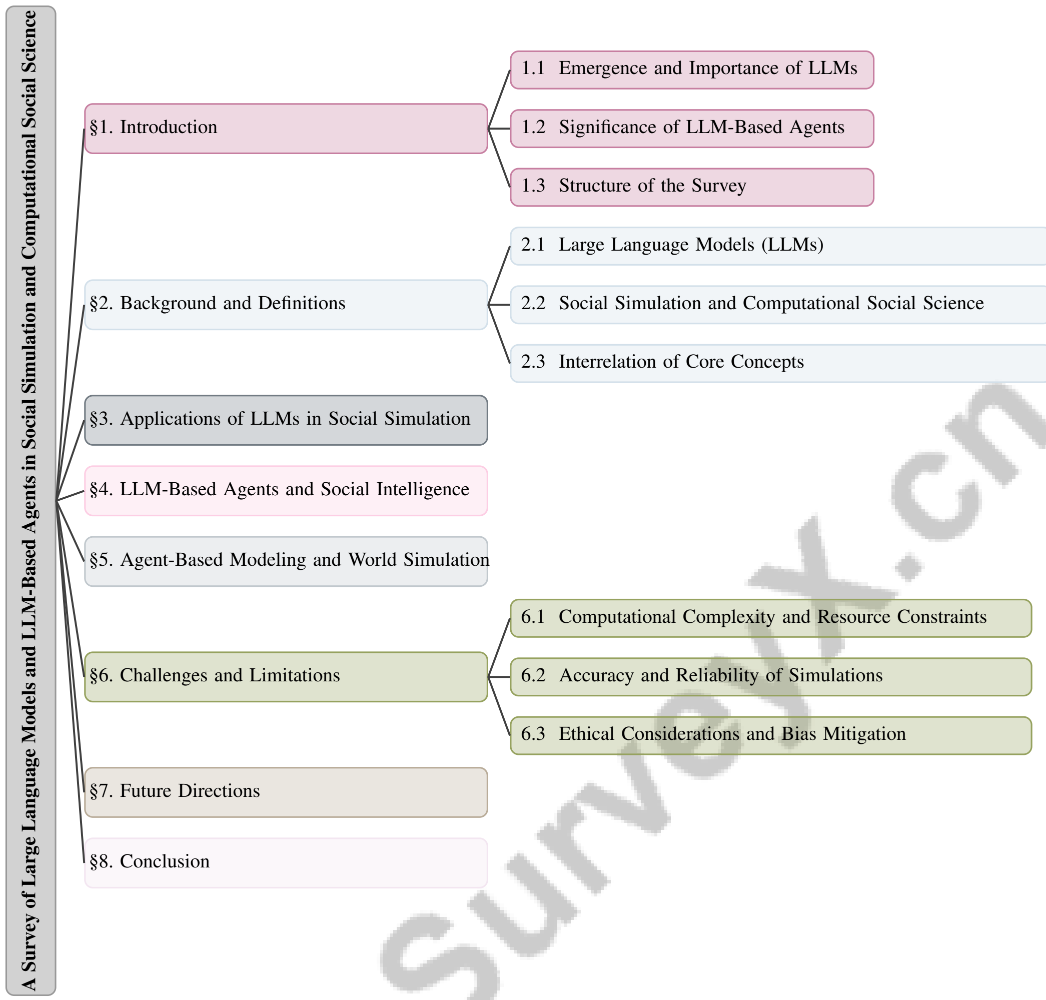

Figure 1: chapter structure

1.2 Significance of LLM-Based Agents

LLM-based agents represent a pivotal advancement in computational social science, fundamentally reshaping social behavior simulation. These agents leverage LLM capabilities to replicate human-like interactions, providing nuanced insights into social dynamics across various contexts [9]. The Social-Bench benchmark evaluates the sociality of conversational agents, demonstrating their effectiveness in simulating intricate social interactions [10].

In economic experiments, LLM agents simulate human behavior, yielding fresh insights into decision-making processes [11]. Their application spans individual, scenario, and societal simulations, enhancing the realism of computational models [12]. The dynamics of collaboration and confrontation among LLM agents in gameplay underscore the necessity for comprehensive studies in this domain [13].

The STSS benchmark further elucidates language agents' capabilities by objectively assessing their actions in multi-agent simulations [14]. Additionally, benchmarks evaluating LLMs' performance in social interactions under varying conditions provide essential frameworks for understanding their social capabilities [15]. In gaming, the 'A MONG A GENTS' benchmark assesses LLMs' reasoning and social deduction abilities [16].

LLM-based agents foster spontaneous cooperative behaviors, enhancing simulation authenticity [17]. Incorporating Theory of Mind (ToM) enhances their responsiveness to human needs, improving user interactions [18]. Frameworks like the Social-network Simulation System (S 3) utilize LLM-

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empowered agents to simulate user interactions and emotions, refining social phenomenon modeling [19]. OASIS, a scalable simulator, facilitates large-scale agent interaction exploration [20].

Psychological dimensions of LLMs, evaluated through specific benchmarks, enhance understanding of LLM-based agents' roles in simulations [21]. A human-centered approach to transparency underscores the need to accommodate diverse stakeholder needs, reinforcing the importance of LLM-based agents in computational social science [22]. These advancements highlight the transformative impact of LLM-based agents in enriching social simulations' realism, scalability, and depth.

Moreover, LLM-based agents can enhance predictive analytics by converting qualitative expert insights into quantifiable features [23]. In gaming, LLM-based game agents (LLMGAs) exhibit human-like decision-making, leveraging LLM cognitive capabilities [24]. K-Level Reasoning (K-R) significantly enhances LLMs' strategic reasoning, providing new insights into complex social dynamics [25]. The limitations of existing methods, which focus primarily on text-based interactions among a few agents, necessitate new approaches for simulating dynamic real-world scenarios [5]. The proposed Generative Agent-Based Model (GABM) framework optimizes EV charging behavior by incorporating psychological characteristics and user preferences, exemplifying LLM-based agents' diverse applications [2]. Asynchronous AI agents that process multiple requests concurrently further enhance interactivity and simulation effectiveness [4]. A benchmark for evaluating LLM simulations based on susceptibility to caricature offers researchers a valuable tool for assessing model quality [3].

1.3 Structure of the Survey

This survey is structured to provide a comprehensive overview of LLMs and LLM-based agents in social simulation and computational social science. It begins with an introduction highlighting the emergence and significance of LLMs and LLM-based agents, followed by a background section elucidating core concepts and terminologies associated with LLMs and their applications in simulating social behaviors. Subsequent sections explore specific applications of LLMs, such as virtual persona creation, gaming environments, and conversational AI.

The survey examines how LLM-based agents enhance social intelligence by simulating human interactions and integrating elements of Theory of Mind and moral frameworks. While LLMs can mimic human social interactions, their behaviors stem from learned statistical patterns rather than genuine emotional understanding or cognition. The implications of LLMs possessing a form of Theory of Mind are discussed, particularly regarding their influence on individual and group dynamics in human-agent interactions, including empathy and moral decision-making. The study identifies opportunities and challenges for aligning LLM behaviors with human values, emphasizing the need for further investigation into their alignment with societal norms and ethical considerations [6, 8]. It also addresses the integration of LLMs with agent-based modeling techniques to create sophisticated world simulations, highlighting challenges such as computational complexity and ethical considerations.

Finally, the survey outlines future research directions in this interdisciplinary field, emphasizing advancements in simulation techniques, multimodal integration, and the expansion of applications and evaluation metrics. The conclusion synthesizes essential findings, highlighting the transformative potential of LLMs in computational social science, particularly in text analysis tasks like sentiment analysis and discourse analysis. By leveraging LLMs, researchers can enhance data annotation and analysis efficiency, revolutionizing methodologies within the field. Best practices for utilizing LLMs, including model selection and fine-tuning strategies, are crucial for maximizing their effectiveness in understanding complex social phenomena [26, 27, 28, 7].The following sections are organized as shown in Figure 1.

2 Background and Definitions

2.1 Large Language Models (LLMs)

Large Language Models (LLMs) represent a major leap in artificial intelligence, known for their proficiency in processing and generating human-like text. Models such as GPT and BERT leverage vast datasets and sophisticated deep learning architectures to grasp the nuances of human communication, supporting tasks like text generation, translation, and complex problem-solving [29]. The progression of LLMs from simple text generators to advanced tools capable of modeling intricate social interactions marks a significant shift in their application [30].

In computational social science, LLMs are pivotal for simulating complex social behaviors, offering insights into multifaceted social systems [26]. Their incorporation into frameworks like the Generative Agent-Based Model (GABM) enhances simulations by integrating user preferences and psychological traits, as demonstrated in electric vehicle charging scenarios [29]. The development of large-scale multimodal agents, such as LMAgent, further illustrates LLMs' ability to simulate diverse user behaviors across various contexts, including e-commerce [29].

Despite their capabilities, LLMs face challenges in certain applications. In dynamic environments like Minecraft, they struggle with precise action execution, highlighting inefficiencies in action prediction and strategic reasoning [29]. The phenomenon of hallucinations, where LLMs produce factually incorrect information, complicates their use in critical applications, emphasizing the need for ongoing research into mitigation strategies [29].

LLMs also contribute to the pursuit of Artificial General Intelligence (AGI), particularly in gaming environments where they act as agents capable of human-like decision-making [29]. Their asynchronous capabilities, supported by architectures like ATR, enable effective multitasking and tool usage, enhancing interaction fluidity [29]. As LLMs evolve, their applications in social simulation and computational social science are expected to expand, offering transformative potential for modeling and understanding complex social phenomena.

2.2 Social Simulation and Computational Social Science

Social simulation and computational social science are interdisciplinary fields employing computational methodologies to model and explore social behaviors and interactions. Techniques like agent-based modeling (ABM) simulate interactions of autonomous agents within defined environments to elucidate complex systems dynamics [31]. Traditional ABMs often fall short in capturing human communication intricacies and individual belief diversity, necessitating more sophisticated approaches [32].

Integrating LLMs enhances social simulations' fidelity, enabling modeling of civilization evolution under varied moral frameworks and decision-making processes [33]. This capability is particularly advantageous in strategic simulations, such as Diplomacy, where relationship management, strategic decision-making, and negotiation execution are crucial [34]. Through these applications, LLMs provide nuanced understanding of social dynamics, enriching computational social science.

LLMs also improve political text and data analysis, enhancing predictive accuracy and offering deeper insights in political science, thus broadening social simulation scope [35]. Multi-agent systems illustrate complex social system simulations, focusing on problem-solving and world simulation [36]. These systems model scenarios like international relations and conflict initiation probabilities, providing frameworks for understanding historical and contemporary conflicts [37].

LLMs foster interdisciplinary collaboration, influencing co-authorship and collaboration patterns across fields [38]. This evolution underscores computational social science's significance in examining social behaviors, offering innovative tools and methodologies to explore and analyze human interactions complexities in an increasingly digital landscape. Benchmarks for evaluating social intelligence, including understanding and predicting others' actions and intentions, further emphasize LLMs' relevance in these fields [39]. The diverse applications of LLMs in social scientific tasks, such as humor, offensiveness, sentiment, and emotion, exemplify their broad utility in computational social science [40].

Challenges persist, including ambiguity in social constructs, nuanced social signals, and the need for multi-perspective reasoning, requiring agents to adapt and learn from social contexts [41]. Fragmentation in understanding methodologies across social science fields, exacerbated by the lack of cross-disciplinary communication in word embedding models application, complicates computational social science [42]. The challenge of obtaining accurate statistical estimates using potentially biased or inaccurate LLM annotations further complicates this domain [26]. Nonetheless, LLMs' ongoing evolution and integration into social simulation and computational social science continue to present promising avenues for advancing our understanding of complex social behaviors.

2.3 Interrelation of Core Concepts

Integrating large language models (LLMs), social intelligence, and agent-based modeling (ABM) creates a comprehensive framework significantly enhancing computational social science. LLMs, with advanced natural language processing capabilities, function as both search operators and generators within optimization algorithms, fostering contextually rich interactions in ABM [43]. This synergy addresses traditional models' limitations, which often lack human-like characteristics such as bounded rationality and learning capabilities, enhancing simulations' expressiveness and effectiveness [44].

This interrelation is exemplified by integrating qualitative insights and predictive analytics, highlighting incorporating subjective expert knowledge into standardized quantitative frameworks [23]. This integration is crucial for enhancing social simulations' fidelity and providing a more nuanced understanding of social dynamics.

Moreover, the interplay between LLMs and active learning techniques improves classification performance in resource-constrained environments [45], particularly relevant in multi-agent systems (MASs) strategic interactions. The Extended Coevolutionary (EC) Theory offers a novel perspective by merging concepts from game theory, coevolutionary algorithms, and adaptive learning [46].

LLMs' capabilities are multifaceted, suggesting a granular understanding of their role in social simulations [47]. However, a primary challenge lies in ambiguous outputs that yield vague action descriptions, hindering their ability to predict actions in real-time interactions [48].

The concept of K-Level Reasoning (K-R) organizes reasoning into hierarchical levels and employs recursive mechanisms to enhance LLMs' strategic depth, linking LLMs with strategic reasoning concepts [25]. Additionally, the Social-LLM concept, inspired by social network homophily theory, posits that socially connected users exhibit similarities, enriching user behavior modeling [49].

The CoMPosT framework categorizes LLM simulations based on dimensions such as Context, Model, Persona, and Topic, providing a novel approach to evaluating caricature in simulations [3]. Despite LLMs' high alignment with human behavior in game theory, their capability boundaries remain unclear [50].

Finally, employing LLMs for ideological scaling illustrates the connection between language understanding and the measurement of social constructs, further demonstrating the interrelation of core concepts [30]. Collectively, these advancements underscore the robust foundation established by integrating LLMs, social intelligence, and ABM, facilitating the simulation and analysis of complex human interactions and advancing the field of computational social science.

3 Applications of LLMs in Social Simulation

Large language models (LLMs) are pivotal in social simulation, particularly in crafting virtual personas that enrich the realism and interactivity of simulated environments. This section delves into LLMs' contributions to virtual persona creation and their applications across various domains.

3.1 LLMs in Virtual Persona Creation

LLMs have revolutionized virtual persona creation in social simulations by enabling the development of complex, interactive characters that enhance realism through linguistic nuance capture, facilitating realistic simulations of opinion dynamics [51]. This capability is crucial for understanding intricate social interactions and decision-making, as evidenced by coevolutionary dynamics integration and LLM-based strategy recommendations [46]. The RED-CT methodology exemplifies LLM-generated labels for classifier training, automating persona creation and enhancing adaptability [45].

In gaming environments, LLMs demonstrate human-like reasoning and interaction, as seen in LLMGAs [24]. The LARM model highlights LLMs' capacity to create virtual personas capable of complex environment interactions, processing task descriptions and images to predict actions, enhancing simulation realism [48]. The MEOW framework further utilizes LLMs to simulate communication game behaviors, refining persona representations [1]. Additionally, the Social-LLM approach leverages social network interactions and user profiles for personalized persona creation [49], while LMAgent supports multimodal interactions, enabling autonomous activities like chatting and browsing [5].

LLMs' integration into simulation frameworks, particularly in computational experiments, significantly advances the understanding of complex systems by simulating human-like interactions [29]. The CONFIDENCE-DRIVEN INFERENCE method combines LLM annotations with human input for accurate statistical estimates, reinforcing virtual persona reliability [26]. These advancements underscore LLMs' robust capabilities in virtual persona creation, offering new dimensions for simulating social interactions and insights into complex social dynamics, as illustrated by the LLM-based Ideological Scaling (LLM-IS) method [30].

3.2 LLM-Based Agents in Game Environments

LLMs are increasingly employed in game environments to model complex social behaviors and interactions. LLM-based agents adeptly simulate intricate social dynamics in both competitive and cooperative game genres, aligning closely with human decision-making processes [24]. Their capabilities suggest a strong fit for simulating human-like decision-making within game-theoretic contexts [50].

In strategic games, LLMs demonstrate proficiency in reasoning and decision-making that mirrors human strategies, enhancing the realism and depth of simulations [52]. However, challenges persist, particularly in scenarios requiring complex randomization, where LLMs may not perform optimally [53]. The complexity of these games necessitates sophisticated modeling techniques to accurately capture social interactions and strategic variability.

Integrating LLM-based agents into gaming environments enhances the authenticity of simulations and provides a valuable framework for exploring competition and cooperation dynamics. This capability is essential for developing sophisticated social behavior models, offering insights into agent interactions, negotiation processes, and conflict resolution in virtual settings. Leveraging advancements in topic modeling and socio-cognitive theories from developmental psychology, researchers can better understand how agents navigate cultural contexts, enhancing their ability to simulate complex social interactions in AI systems [54, 55]. As research progresses, LLM-based agents are set to significantly advance our understanding of social behaviors in game environments and contribute to the broader field of computational social science.

3.3 Conversational AI and Language Style Simulation

The application of LLMs in simulating conversational AI and language styles marks a significant advancement in artificial intelligence, providing a robust framework for understanding and replicating human communication. The Community Alignment Framework (CAF) generates high-fidelity digital representations of online communities, effectively simulating community interactions [56]. This approach underscores LLMs' potential to capture the dynamics of conversational exchanges, creating more authentic virtual environments.

The integration of LLMs with localized social network interactions, as demonstrated by the Social-LLM method, enhances user behavior modeling by addressing user detection challenges [49]. This method leverages LLM capabilities to simulate complex social interactions on digital platforms, deepening the understanding of user dynamics.

Moreover, combining LLM annotations with human input based on confidence levels optimizes statistical estimates, enhancing the reliability of conversational AI systems [26]. This integration emphasizes the importance of human oversight in AI-driven simulations for accuracy and credibility.

Recent advancements in LLMs demonstrate their capacity to enhance conversational AI and mimic diverse language styles, providing innovative tools for examining human communication intricacies in virtual environments. These models facilitate engagement-driven content generation within social networks and transform text analysis across social science applications, making tasks like sentiment analysis and political discourse identification more accessible. Furthermore, interdisciplinary collaboration in LLM research highlights their potential to address complex scientific challenges, while ethical considerations underscore the importance of accountability and bias mitigation in shaping the future of AI-driven communication [7, 57, 58, 59, 38]. As LLMs evolve, their role in enhancing conversational simulations is poised to expand, significantly contributing to the broader field of computational social science.

4 LLM-Based Agents and Social Intelligence

LLM-based agents are pivotal in replicating complex human-like interactions and decision-making processes, thereby enhancing social intelligence in simulations. This section explores the methodologies and frameworks that empower these agents to emulate human behavior, improving the authenticity of social dynamics in virtual environments. As illustrated in Figure 2, the hierarchical structure of LLM-based agents plays a crucial role in this enhancement of social intelligence. The figure categorizes advancements in simulation, cognitive enhancements, adaptability, and ethical reasoning, emphasizing how these agents integrate Theory of Mind and moral frameworks to mimic human-like interactions. The subsequent subsection discusses the mechanisms through which LLMs achieve this mimicry, highlighting advancements in their design and functionality.

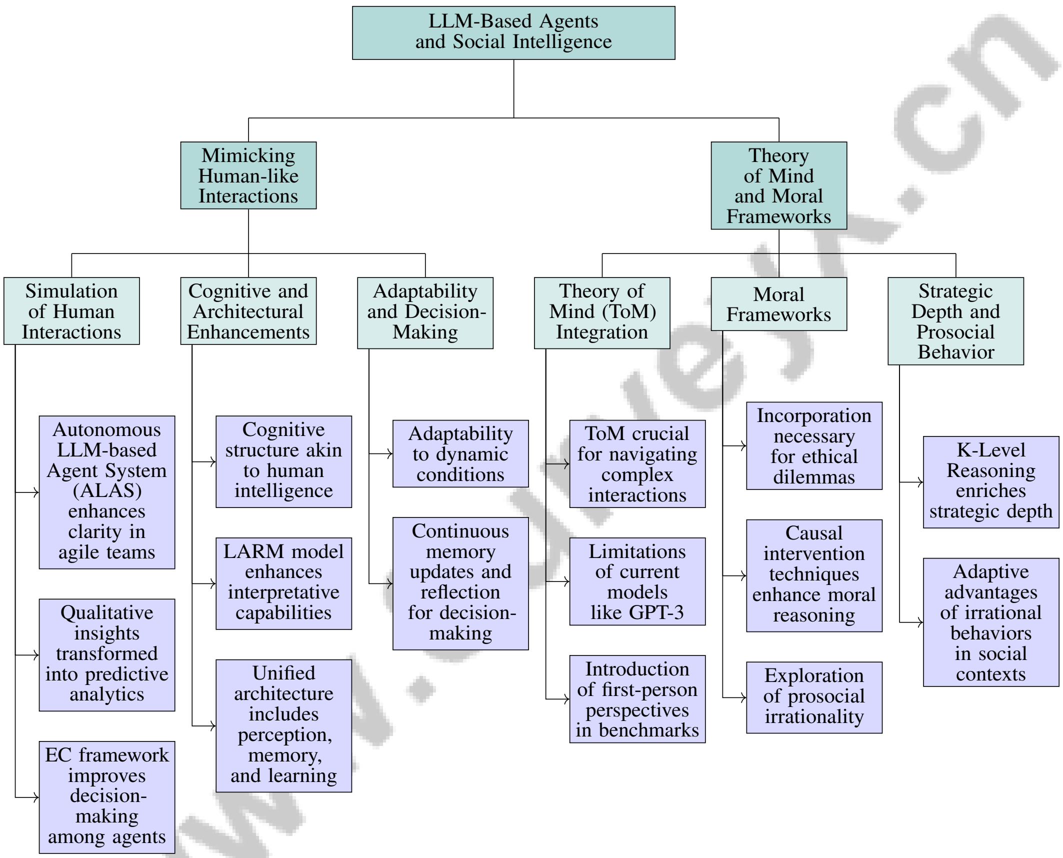

Figure 2: This figure illustrates the hierarchical structure of LLM-based agents and their role in enhancing social intelligence, focusing on mimicking human-like interactions and integrating Theory of Mind and moral frameworks. It categorizes advancements in simulation, cognitive enhancements, adaptability, and ethical reasoning, highlighting the potential of LLMs to emulate complex social behaviors and decision-making processes.

4.1 Mimicking Human-like Interactions

LLM-based agents have significantly advanced in simulating human-like interactions and decision-making, crucial for understanding social dynamics in virtual environments. The Autonomous LLM-based Agent System (ALAS) exemplifies how these agents enhance clarity and alignment in agile teams by refining user stories [60], showcasing their potential to simulate intricate social interactions. Furthermore, LLMs transform qualitative insights into quantifiable metrics, translating expert intuition into predictive analytics, which enhances predictive accuracy in simulating realistic social interactions and opinion dynamics [23, 51]. The EC framework elucidates cooperation and defection dynamics, improving decision-making among agents [46].

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The cognitive structure of LLMs, akin to human intelligence, underscores their potential for nuanced understanding and communication in simulations [47]. Models like LARM enhance interpretative capabilities by predicting subsequent actions, bolstering social intelligence in simulations [48]. The unified architecture for LLM-based game agents (LLMGAs) includes perception, memory, thinking, role-playing, action, and learning components, facilitating human-like decision-making [24]. The MEOW framework exemplifies LLM applications that enhance reasoning abilities in data-scarce environments [1], while LMAgent improves user behavior simulations by replicating complex human social interactions [5].

LLM-based methods' effectiveness lies in their adaptability to dynamic conditions and user expectations, utilizing continuous memory updates and reflection for enhanced decision-making [2]. Collectively, these advancements illustrate the significant impact of LLM-based agents in mimicking human-like interactions, offering new dimensions for exploring complex social behaviors within virtual environments. As LLMs evolve, their ability to enhance simulation fidelity and depth is poised to contribute meaningfully to computational social science.

4.2 Theory of Mind and Moral Frameworks

Integrating Theory of Mind (ToM) and moral frameworks into LLM-based agents marks a significant advancement in social intelligence within simulations. ToM, the ability to infer others' mental states, is crucial for developing agents capable of navigating complex social interactions. Current models like GPT-3 highlight limitations in achieving nuanced social intelligence, emphasizing the need for sophisticated approaches to incorporate ToM capabilities into LLMs [61].

The SOTOPIA framework combines behavior cloning with self-reinforcement training, enabling LLMs to learn from expert models and their interactions, thus enhancing human-like reasoning and decision-making [62]. This approach fosters the development of agents that adapt to dynamic social environments by learning from past experiences.

Incorporating moral frameworks is essential for ensuring that LLM-based agents can navigate ethical dilemmas and align with human values. A psychological perspective on moral dilemmas integrates insights from sociology, providing a comprehensive understanding of the challenges LLMs face in moral reasoning [63]. Techniques for causal intervention in LLMs further enhance the exploration of moral frameworks, allowing for nuanced assessments of ethical dilemmas [17].

Introducing first-person perspectives in ToM benchmarks provides unique scenarios reflecting real-world social interactions, allowing for more accurate assessments of LLMs' social intelligence capabilities [64]. Additionally, K-Level Reasoning (K-R) enables LLMs to form higher-order beliefs about others' beliefs, enriching the strategic depth of these models in social simulations [25].

Exploring prosocial irrationality within LLMs, rooted in evolutionary sociology, illustrates the adaptive advantages of incorporating irrational behaviors in social contexts [65]. This perspective enhances understanding of how LLM-based agents can simulate human-like interactions that reflect both rational and irrational elements of social behavior.

The integration of ToM and moral frameworks into LLM-based agents signifies a crucial evolution in AI systems capable of simulating human-like social intelligence. This evolution improves agents' ability to understand and respond to users' mental and emotional states, opening new avenues for investigating complex social dynamics in virtual environments. Employing LLMs in diverse scenarios allows researchers to analyze how these agents exhibit prosocial behaviors, navigate ethical dilemmas, and adapt decision-making processes to reflect human-like reasoning. These efforts underscore the potential for LLMs to contribute meaningfully to our understanding of social phenomena while raising important questions about their alignment with human values in real-world applications [17, 6, 5, 8, 66].

As shown in Figure 3, the study of LLM-based agents and their capacity for social intelligence involves exploring complex concepts such as the theory of mind and moral frameworks. This exploration is vividly depicted through a series of illustrative figures that provide insights into various cognitive biases, the accuracy of social intelligence assessments, and the intricacies of experimental design. One image categorizes cognitive biases into six distinct groups, each represented with engaging visuals and thought-provoking questions, highlighting their influence on decision-making and social behavior. Another chart presents a comparative analysis of Social IQa accuracy among different

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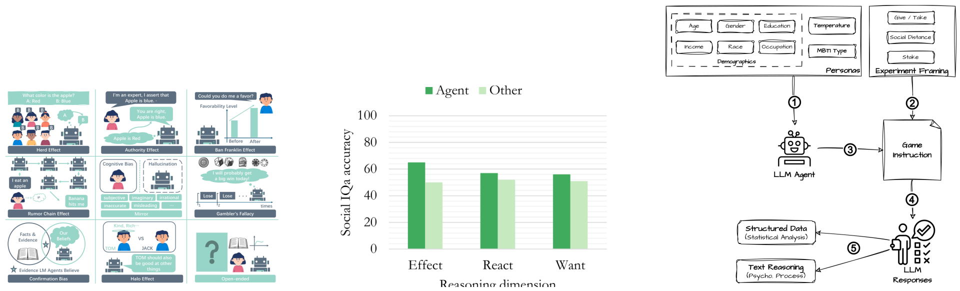


(a) The image illustrates various cognitive biases and their effects on decision-making and social behavior.[65]

(b) Social IQa accuracy[61]

(c) An Experiment Design Flowchart[66]

Figure 3: Examples of Theory of Mind and Moral Frameworks

groups, emphasizing reasoning's role in social intelligence. Additionally, a detailed flowchart outlines the experimental design process, focusing on demographic variables that shape fictional personas for research purposes. Together, these visual aids lay the groundwork for understanding how LLM-based agents can emulate human-like social understanding and moral reasoning, paving the way for more nuanced and ethically aware artificial intelligence systems [65, 61, 66].

5 Agent-Based Modeling and World Simulation

Category	Feature	Method
Integration of LLMs with Agent-Based Modeling Frameworks	Multimodal Integration LLM-Driven Interactions	LARM[48] SCS[67], SABM[68]
Enhancing Realism and Complexity in Simulations	Reasoning and Strategy Agent Interaction Input Integration Task Management	K-R[25] MEOW[1] LMA[5] ATR[4]

Table 1: This table presents a summary of methods integrating large language models (LLMs) with agent-based modeling frameworks. It highlights key features and methodologies used to enhance simulation realism and complexity, facilitating advanced interactions in virtual environments.

The integration of large language models (LLMs) into agent-based modeling (ABM) systems marks a significant advancement in computational social science, enhancing simulation capabilities to explore social dynamics with greater depth. Table 1 provides a comprehensive overview of various methods utilized for integrating large language models with agent-based modeling frameworks, emphasizing their role in enhancing realism and complexity in simulations. Table 3 provides a comprehensive comparison of various methods for integrating large language models (LLMs) with agent-based modeling frameworks, focusing on their integration approaches, simulation capabilities, and adaptability characteristics. This section examines how LLMs enrich ABM frameworks, emphasizing their role in augmenting simulation realism and complexity.

5.1 Integration of LLMs with Agent-Based Modeling Frameworks

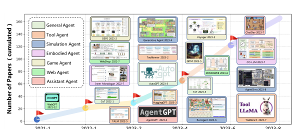
Method Name	**Integration Approach**	**Simulation Capabilities**	**Agent Adaptability**
SABM[68]	Historical Context Interactions	Real-world Systems	Adapt Their Strategies
LARM[48]	Textual And Visual	Real-time Decision-making	Dynamic Social Contexts
MEOW[1]	Generative Agents-based	Complex Human Systems	Dynamic Social Contexts
LMA[5]	Multimodal Llms	Complex User Behaviors	Dynamic Social Contexts
SCS[67]	Historical Context	Complex Social Phenomena	Adapt Their Strategies

Table 2: Comparison of Integration Approaches and Capabilities of Various Methods in Agent-Based Modeling with LLMs. The table summarizes the integration strategies, simulation capabilities, and agent adaptability of five distinct methods, showcasing their unique contributions to enhancing agent interactions in virtual environments.

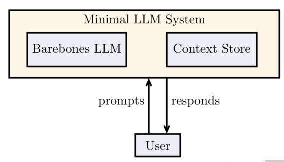
Integrating LLMs with ABM frameworks significantly enriches simulations by leveraging LLMs' linguistic and cognitive capabilities to enhance agent interactions in virtual environments, offering nuanced insights into social phenomena. The S3 simulation system exemplifies this integration by using LLM-empowered agents to model user interactions in social networks, capturing information, emotion, and attitude dynamics [19]. Smart Agent-Based Modeling (SABM) utilizes LLMs to simulate real-world systems, allowing agents to interact based on historical context, thereby enhancing simulation authenticity and adaptability [68].

The LARM framework integrates LLMs with ABM by incorporating textual and visual inputs, enhancing simulations for real-time decision-making in complex environments [48]. This approach enables agents to adapt behaviors in response to evolving social contexts, improving simulation fidelity. The MEOW framework uses generative agents-based simulation to train expert models, assisting LLMs in reasoning tasks, highlighting LLMs' versatility in modeling diverse social scenarios and enhancing strategic interactions among agents [1].

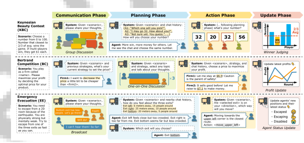
LMAgent dynamically generates multimodal prompts and processes information efficiently, allowing agents to simulate real-user behaviors in complex social environments [5]. These advancements demonstrate LLMs' potential to enhance ABM frameworks, offering scalable, realistic simulations. As LLMs advance, their integration into computational social science is expected to deepen our understanding of complex social phenomena, streamlining research methodologies and providing insights into social dynamics and trends [27, 7].



(a) An Overview of Agent Research in the Past Year[69]



(b) Minimal LLM System[70]



(c) Communication, Planning, Action, and Update Phases in a Multi-Agent System[67]

Figure 4: Examples of Integration of LLMs with Agent-Based Modeling Frameworks

As illustrated in Figure 4, the integration of LLMs with ABM frameworks signifies a major advancement in AI, facilitating world simulation and sophisticated agent systems development. The examples highlight agent research diversity, minimal LLM system architecture, and multi-agent system phases, demonstrating LLMs' potential to enhance agent-based modeling for nuanced, interactive simulations of complex systems [69, 70, 67]. Additionally, Table 2 provides a comprehensive comparison of different methods that integrate Large Language Models (LLMs) with Agent-Based Modeling (ABM) frameworks, highlighting their approaches, simulation capabilities, and adaptability characteristics.

5.2 Enhancing Realism and Complexity in Simulations

Integrating LLMs into simulation frameworks significantly enhances the realism and complexity of agent-based models, providing nuanced insights into social dynamics. LLMs' advanced natural language processing enables sophisticated virtual environments where agents engage in complex interactions, improving simulation fidelity. The Generative Agent-Based Model (GABM) exemplifies this by simulating behaviors such as electric vehicle charging, incorporating user preferences and psychological traits [29].

Asynchronous capabilities in LLMs facilitate real-time interactions and multitasking, enhancing simulations' responsiveness and interactivity [4]. Multimodal inputs, as demonstrated by frameworks like LMAgent, allow agents to process diverse information sources, creating immersive simulations where agents exhibit human-like reasoning and decision-making [5]. K-Level Reasoning (K-R) in LLMs adds complexity by organizing reasoning hierarchically, enhancing strategic depth in agent interactions [25].

Frameworks like MEOW, employing generative agents-based simulation for expert model training, exemplify LLMs' potential to enhance learning and adaptation within simulations [1]. These advancements underscore LLMs' transformative impact, allowing researchers to explore intricate social phenomena with greater depth, revealing insights into opinion dynamics, user engagement, and collective behaviors in various contexts [71, 5, 27, 58, 72]. As LLMs evolve, their role in advancing computational social science is poised to significantly enhance our understanding of complex social dynamics and interactions.

Feature	S3 Simulation System	Smart Agent-Based Modeling (SABM)	LARM Framework
Integration Approach	Llm-empowered Agents	Historical Context	Textual And Visual Inputs
Simulation Capability	User Interactions	Real-world Systems	Real-time Decision-making
Adaptability Characteristics	Emotion Dynamics	Simulation Authenticity	Behavior Adaptation

Table 3: This table presents a comparative analysis of three agent-based modeling frameworks—S3 Simulation System, Smart Agent-Based Modeling (SABM), and LARM Framework—highlighting their integration approaches, simulation capabilities, and adaptability characteristics. The comparison underscores the diverse methodologies employed to enhance realism and interactivity in simulations through the integration of large language models (LLMs).

6 Challenges and Limitations

The deployment of large language models (LLMs) in computational social science presents a complex landscape of challenges and limitations that must be addressed to enhance their effectiveness. Key issues include computational complexity and resource constraints, which not only impede the efficiency of simulations but also affect the fidelity of their outcomes. Understanding these challenges is crucial for advancing the application of LLMs in this field.

6.1 Computational Complexity and Resource Constraints

Integrating LLMs into simulations introduces substantial computational challenges and resource constraints, as seen in generative-agent-based simulations like the MEOW framework, which incur significant operational costs [1]. The recursive mechanisms in approaches like K-Level Reasoning (K-R) further escalate computational demands, impacting scalability [25]. Managing state transitions and events in asynchronous environments complicates consistency maintenance during high-frequency interactions, crucial for dynamic simulations [4]. Moreover, scalability issues in network representation methods require extensive computational resources, limiting LLMs' application in user behavior modeling [49].

Simulation accuracy relies heavily on input data quality and diversity, which significantly influence the realism of simulated behaviors [5]. Insufficient or extreme data can compromise accuracy, highlighting the need for robust data collection and preprocessing [2]. Existing benchmarks often focus on replicating known behaviors, falling short in evaluating open-ended responses' quality, thus limiting insights into human behavior [3]. Disparities between LLM performance and human capabilities necessitate cautious integration into social science research, as significant differences in performance metrics can undermine simulation outcomes' validity [50]. Despite technological advancements, limitations in representing human-like characteristics and the need for improved explainability persist, hindering LLMs' effectiveness in simulations [29].

Addressing these computational challenges and resource constraints is vital for advancing computational social science. Future research must focus on developing efficient architectures and methodologies for LLM deployment, particularly in navigating user engagement and opinion dynamics within social networks. Leveraging reinforcement learning and adaptive frameworks can enhance LLM capabilities, fostering meaningful content generation and maximizing user interaction, leading to more robust applications in this domain [7, 58].

6.2 Accuracy and Reliability of Simulations

Ensuring accuracy and reliability in LLM-based simulations is a critical concern, as these models often struggle to replicate the complexities of human interactions. Inherent biases and inaccuracies within LLMs can yield outputs divergent from authentic human responses [30], compounded by input data quality reliance [73]. The complexity of extracting linguistic features from LLMs further complicates accuracy assessment [74]. Simulations often represent simplified real-world systems, compromising result reliability [46]. Current studies are limited by pre-existing knowledge embedded in LLMs, impacting overall simulation accuracy [24]. Additionally, LLMs' potential to generate inaccurate and biased annotations poses significant risks, as these inaccuracies can lead to misleading conclusions if not properly managed [26].

LLMs' unique characteristics, including their scale and autoregressive nature, present analytical challenges compared to traditional deep learning models [75]. Task-specific fine-tuned models have shown superior performance in zero-shot settings, highlighting the importance of prompting strategies on classification outcomes [76]. Sensitivity to prompt design can lead to task misunderstandings, complicating simulation reliability. In therapeutic contexts, ensuring coherent and empathetic LLM responses remains challenging, indicating ongoing issues with accuracy and reliability in sensitive applications [60]. The applicability of human psychometric tests to LLMs also raises concerns about the reliability of self-reported assessments [21]. A lack of robust qualitative assessments often results in an incomplete understanding of LLM intelligence and its implications [77].

LLM agents' propensity to converge towards factual information can lead to simulations failing to accurately represent individuals with resistant viewpoints [51]. Additionally, accuracy and reliability issues related to LLM-generated labels, especially concerning biases, can compromise training data quality [45], leading to skewed representations of social phenomena and affecting simulation validity. Addressing these issues is essential for advancing LLM-based simulations in computational social science, facilitating the establishment of standardized best practices and enhancing LLMs' effectiveness in various text analysis tasks, including sentiment analysis and political discourse identification. Developing robust models and methodologies that account for social complexities and biases will be crucial for improving the fidelity and applicability of these simulations in capturing the intricacies of human social behaviors [27, 7].

6.3 Ethical Considerations and Bias Mitigation

The integration of LLMs in social simulations requires thorough examination of ethical considerations and bias mitigation strategies to ensure equitable and accurate outcomes. Inherent biases in LLM training data can lead to unintended consequences in encoding diverse human values [17]. The potential for LLMs to perpetuate existing biases is particularly pronounced due to their reliance on historical data, which may inadequately represent diverse demographic perspectives [71]. This issue is further exacerbated by LLMs' tendency to exhibit WEIRD (Western, Educated, Industrialized, Rich, and Democratic) biases, often failing to capture non-Western and older populations' moral values and decision-making processes [78].

Addressing these concerns necessitates interdisciplinary collaboration among ethicists, technologists, and policymakers to establish comprehensive ethical guidelines that align LLMs with diverse stakeholder needs [79]. The importance of ethical practices in Social-AI research is underscored by advocacy for participatory approaches involving diverse stakeholders, ensuring alignment with societal needs and values [41]. Such approaches are crucial for mitigating biases and promoting ethical AI deployment. The introduction of benchmarks like CHAST highlights readiness issues of LLM-powered applications in sensitive contexts, such as recruitment, underscoring the necessity for further research in understanding and mitigating biases in AI [78]. Findings from the CoMPosT framework reveal significant disparities in susceptibility to caricature across different demographics and topics, emphasizing the need for careful evaluation and documentation in LLM simulations [3].

The ethical implications of deploying LLMs as substitutes for human participants must be scrutinized, recognizing the historical context of demographic representation and exercising caution to avoid potential misuse [80]. Risks associated with LLMs, such as user manipulation and harmful social connections, underscore the importance of aligning LLMs with human values while minimizing harm [43]. Furthermore, the lack of explainability in LLM outputs presents challenges for their deployment in sensitive applications, highlighting the need for transparency and reproducibility in LLM development and deployment [49]. Future research should aim to extend benchmarks to include additional annotation tasks and datasets, refining validation workflows to ensure the accuracy and reliability of simulations [76].

AI-generated, for reference only.

7 Future Directions

Exploring future directions for large language model (LLM)-based simulations necessitates focusing on advancements that will propel the field forward. Enhancing simulation and interaction techniques is critical for increasing the realism and applicability of these models across various domains. This section discusses specific advancements in these techniques, emphasizing their role in improving agent adaptability and enriching the depth of social dynamics within LLM-based frameworks.

7.1 Advancements in Simulation and Interaction Techniques

The evolution of advanced simulation and interaction techniques in LLM-based simulations is essential for enhancing realism and applicability. Integrating hybrid models that combine LLMs with reinforcement learning enhances agent adaptability in dynamic environments and simulates complex social interactions [60]. Future research should refine LLM-based feature encoding techniques to bolster predictive analytics, ensuring simulations remain accurate and contextually relevant [23]. Optimizing task distribution strategies and algorithm adaptability across various data types is crucial for aligning advancements in simulation techniques with real-world applications [45]. Such enhancements will enable more precise simulations, facilitating new dimensions for exploring user interactions in diverse settings.

In negotiation dynamics, refining personality trait definitions in AI agents and examining negotiations with symmetric preference profiles is vital to understanding their impact on outcomes [51]. Developing efficient evaluation methods and exploring additional dimensions of social intelligence are critical for reducing reliance on human annotators and enhancing the assessment of LLMs' social capabilities [41]. Integrating LLMs in social simulations requires robust evaluation frameworks to explore their capabilities in various social contexts while addressing ethical concerns [43]. Enhancing platforms with simulation acceleration strategies and adaptive self-correction mechanisms will be crucial for advancing the effectiveness and reliability of LLM-based simulations [75].

Further advancements in emotional sensitivity and the potential for LLMs to create original metaphors could enhance the authenticity of simulations, providing deeper insights into human-like interactions. Future research should also explore broader participant demographics and investigate the generalizability of findings across different LLMs, considering alternative interaction modalities to expand the applicability of simulation techniques [76]. These advancements promise to elevate LLM-based simulations significantly, offering new insights into the intricacies of social dynamics and interactions. As research evolves, these innovative techniques will contribute to developing more sophisticated and realistic simulation models, enhancing our understanding of complex social phenomena. Future research directions include improving grounding techniques for LLMs and enhancing simulations of social interactions among agents [24]. Optimizing the computational efficiency of K-Level Reasoning (K-R) and its application in diverse strategic scenarios is crucial for advancing simulation techniques [25]. Enhancing precision by incorporating higher-order proximities and developing sophisticated user feature representations will further improve simulation accuracy [49]. Additionally, future research should focus on refining prompts for elicitation and exploring LLM capabilities in measuring complex constructs [30].

7.2 Integration with Multimodal and Interdisciplinary Approaches

Integrating LLMs with multimodal and interdisciplinary approaches represents a frontier in enhancing their capabilities across diverse fields. Multimodal integration combines textual, visual, and auditory data to create more holistic and contextually rich simulations, improving the realism of LLM-based models [49]. Frameworks like LMAgent exemplify LLMs' potential to process and respond to multimodal inputs, enabling agents to engage in activities such as chatting, browsing, and product reviews in ways that closely mimic human behavior [5].

Interdisciplinary approaches extend LLM utility by incorporating insights from psychology, sociology, and cognitive science, enriching the understanding of social dynamics and interactions [41]. This cross-disciplinary collaboration facilitates the development of sophisticated models that simulate complex human behaviors, providing valuable frameworks for analyzing social phenomena in virtual environments [43]. The integration of LLMs with multimodal and interdisciplinary approaches underscores the need for robust evaluation frameworks to assess model effectiveness in capturing human interaction intricacies across contexts [43]. By leveraging diverse data sources and methodologies, researchers can enhance the accuracy and reliability of LLM-based simulations, paving the way for comprehensive analyses of social behaviors.

Future research should optimize LLM integration with multimodal inputs and interdisciplinary methodologies to expand model applicability. This includes simulating a wider range of social interactions and refining evaluation techniques to ensure fidelity and robustness in simulations [49]. As these advancements unfold, integrating LLMs with multimodal and interdisciplinary approaches promises to significantly enhance computational social science, offering new insights into the complexities of human social dynamics.

7.3 Expanding Applications and Evaluation Metrics

Benchmark	Size	Domain	Task Format	Metric
LLMs4OL[81]	3,000,000	Ontology Learning	Term Typing	MAP@1, F1-score
LM-Coding[82]	30,034	Political Science	Text Classification	F1-score, ICC
LLM-Rep[83]	82,870	Psychology	Replication OF Psychological Experiments	Replication Rate, Effect Size
CSS-PD[84]	362,928	Computational Social Science	Multi-class Classification	Accuracy, Compliance
SOTOPIA[85]	90	Social Intelligence	Role-playing Interactions	Goal Completion, Believability
STSS[86]	325	Social Intelligence	Conversation	Goal Achievement, Summary-Level Evaluation
SESI[87]	1,000	Social Intelligence	Multiple-choice Question Answering	Exact Match
AgentSense[88]	1,225	Social Intelligence	Multi-turn Interaction	PSI, Acc

Table 4: This table provides a comprehensive overview of representative benchmarks used in evaluating large language models (LLMs) across various domains. It details the size, domain, task format, and evaluation metrics for each benchmark, highlighting the diverse applications and methodologies employed in LLM assessments. Such benchmarks are crucial for advancing the understanding and development of LLM capabilities in complex human systems.

Expanding applications and evaluation metrics for LLM-based simulations presents a promising avenue for enhancing their utility across diverse domains. Future research should improve robustness in the simulation process, address LLM reasoning limitations, and explore broader applications of frameworks like MEOW in complex human systems [1]. This enhancement could yield models capable of capturing social dynamics complexities in virtual environments. Exploring complex games and the role of LLMs as multi-agents, coupled with targeted training processes, could significantly enhance decision-making abilities [50].

Emerging trends in interdisciplinary applications, such as computational creativity, robotics, and drug design, highlight LLMs' potential to transcend traditional boundaries and provide innovative solutions. In historical simulations, improving model accuracy and broadening scenario ranges can enhance understanding of intricate diplomatic dynamics. This approach facilitates nuanced analyses of international conflicts, such as those seen in World Wars I and II and the Warring States Period in Ancient China, leveraging advanced AI techniques to uncover patterns that inform conflict resolution and peacekeeping strategies [37, 72, 35].

Developing better evaluation metrics is crucial for assessing LLM thought competence and understanding their implications in real-world applications. This includes mitigating algorithmic bias, enhancing interpretability, and exploring the impact of AI-driven insights on political processes and public policy. Expanding LLM applications in therapeutic contexts, particularly through strategic prompt engineering, could significantly enhance AI-driven mental health interventions. Recent research indicates that effective prompt engineering can improve Problem-Solving Therapy (PST) delivery by LLMs, especially in symptom identification and personalized goal setting, addressing the global shortage of mental health professionals [23, 60, 89, 57].

To enhance understanding of user interactions within social movements, future research should broaden datasets to encompass diverse social movements and refine models like the hybrid HiSim framework, which combines LLMs and agent-based modeling to replicate user response dynamics on platforms like Twitter. This will facilitate accurate simulations and evaluations, improving forecasting of societal impacts [72, 90, 55, 42]. Addressing diverse dialogue contexts and improving robustness against unpredictability caused by self-emotion are critical areas for exploration, alongside ethical considerations in deploying such agents.

Finally, developing standardized benchmarks for evaluating cooperative behaviors in social simulations is essential for advancing the field. By investigating various LLMs and enhancing evaluation metrics like the TRUSTSIM dataset, researchers can improve the reliability and robustness of LLM-based simulations. This refinement addresses inconsistencies in simulated roles and facilitates the development of adaptive algorithms like AdaORPO to optimize performance across social contexts. Consequently, these advancements will enable LLMs to provide deeper insights into the intricate dynamics of human social interactions, transforming the landscape of computational social science and engagement-driven content generation [58, 7, 71]. Table 4 presents a detailed summary of key benchmarks employed to evaluate large language models (LLMs) in different domains, illustrating the expanding applications and evaluation metrics pertinent to LLM-based simulations.

8 Conclusion

This survey has explored the profound influence of large language models (LLMs) and LLM-based agents on the fields of social simulation and computational social science. Through the integration of LLMs with agent-based modeling frameworks, researchers have significantly advanced the realism and intricacy of simulations, leading to a more nuanced understanding of social dynamics. The collaborative abilities of LLM agents, as demonstrated in recent research, underscore their potential to enhance task completion in complex projects by employing effective augmentation strategies.

LLMs have proven adept at replicating human-like interactions and decision-making processes, resulting in the creation of sophisticated models that intricately represent human behavior. Their diverse applications, ranging from virtual persona creation and gaming environments to conversational AI, highlight their adaptability in modeling various social contexts. Moreover, the incorporation of Theory of Mind and moral frameworks into LLM-based agents has substantially augmented their social intelligence, equipping them to adeptly handle intricate interactions and ethical challenges.

The deployment of topic models, such as Structural Topic Modeling (STM), has emerged as a potent technique for text data analysis, empowering social scientists to investigate latent variables and causal relationships within large datasets. This capability is essential for the advancement of computational social science, offering innovative methodologies for examining complex social phenomena.

Despite these advancements, challenges remain, including computational complexity, resource limitations, and ethical considerations. Addressing these challenges is imperative for the continued progress and application of LLM-based simulations. Future research should focus on refining simulation techniques, embracing multimodal and interdisciplinary approaches, and broadening applications and evaluation metrics to ensure the sustained evolution and efficacy of LLMs in social simulation.

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