Beyond the Surface: Navigating Complex Systems via ABMs and Hypergraphs

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Abstract. Interactions, organization, and emergent behaviors are fundamental to all complex systems. These characteristics can be observed in every real-world scenario, prompting the question: how do these interactions among elements serve as the foundation of complex systems? Over the years, researchers have developed various methods to answer such a question. One widely used bottom-up approach is agent-based simulation, which deduces a system's properties by examining its components. Alternatively, a system can be modeled via a top-down approach, such as hypergraphs, mathematical structures abstracting higher-order interactions. These two methods provide different perspectives on the same system, each offering unique and valuable insights. In this Ph.D. project, my primary focus is on social systems, aiming to shed light on the dynamics of group behaviors in online social media.

Keywords: Complex systems · Hypergraphs · ABMs · Stance detection · LLM · Social networks.

1 Introduction

Many closely interconnected components constitute various natural, social, and artificial structures, giving rise to unintelligible behaviors if we focus on a single component at a time [25]. Such organizations are commonly referred to as complex systems, and as examples, we can name traffic control, weather forecast, or policy-making. Usually, the analysis of complex systems involves creating a model that can replicate the real system. These models are typically the result of the collaborative efforts of multiple experts from various fields. Complex systems are characterized by key features such as non-linearity (when small changes in one part of the system can lead to disproportionately large and unpredictable effects in other parts), self-organization, and adaption [8]. Investigating these phenomena means dealing with the following challenges:

- *Data complexity and access*: Complex systems often require and generate vast amounts of data, making analysis and interpretation challenging. Further, online platforms frequently deny or hide their data behind paywalls, making data acquisition difficult.
- *Modeling complexity*: Developing accurate mathematical or computational models for complex systems can be difficult due to their non-linear and dynamic nature.

- *Computational resources*: Simulating or analyzing complex systems may require significant computational resources regarding time, money, and equipment.
- *Interdisciplinary nature*: Understanding complex systems often requires knowledge and cooperation from multiple domain experts.

During my Ph.D. project, I have been focusing on studying social systems, particularly by analyzing social media platforms. Among these platforms, Reddit stands out as a prominent example of an online social data source. Due to the richness and quality of its data, Reddit has become a key resource for researchers who have extensively studied its data to validate various social science theories. While analyzing user behavior in online forums like Reddit sheds light on the fundamental processes through which groups of individuals develop collective thought, it also has significant practical applications, such as enhancing user experience, increasing engagement, and automatically detecting bullying in online conversations [10].

Researchers can use top-down strategies, bottom-up strategies, or a combination of both to understand the intricacies of human behavior. These approaches are complementary and offer different perspectives on the systems to study.

The bottom-up approach involves examining individual components within the complex system and understanding its behavior starting from its basic elements. Agent-based models (ABMs) represent a robust modeling technique that uses such an approach [14]. Specifically, in ABMs, modelers define agents and environments to replicate specific aspects or properties of the underlying reality. These models provide a detailed understanding of how local interactions give rise to system-level behavior, offering fine-grained control and manipulation of individual components. This approach is particularly useful when the behavior of individual elements within the system is well understood.

The top-down approach involves examining the system's global behavior and properties and then deconstructing and understanding the underlying components and interactions. One of the most expressive mathematical structures capable of capturing high-order interactions is a hypergraph, a generalization of a graph where a (hyper)edge connects an arbitrary number of nodes [9]. Hypergraphs are useful for modeling complex systems as they can represent relationships that involve multiple entities simultaneously, unlike graphs, which only model pairwise interactions. Hypergraphs are particularly valuable when examining social networks, as interactions often occur in groups of different sizes. For instance, users might collaborate in teams, participate in group activities, form communities, or work together towards a common goal. All these activities involve more complex connections than simple pairwise relationships. By using hypergraphs, we can more accurately capture and analyze the dynamics of these high-order interactions, leading to better insights and understanding of the system's behavior and structure [41].

Social interactions on online platforms frequently involve written communications. Textual messages can carry multiple meanings, and the context in which they are located can significantly affect their interpretation and nuance. As a result, understanding the semantics of these interactions is crucial and cannot be ignored when examining online user behavior. As technology advances, recent research has proved how the rapid development of large language models (LLMs) has assisted researchers in performing various tasks across multiple fields [39]. After being pre-trained on extensive text corpora, LLMs exhibited vast context-aware knowledge and exceptional semantic comprehension capabilities [12]. For instance, LLMs have demonstrated their effectiveness in stance detection tasks, showing adaptability across different datasets with various prompting schemes and even outperforming supervised models in terms of performance while using fewer resources [15].

My Ph.D. project fits this broader context and has a dual focus. First, it aims to advance the analysis of complex systems by improving ABM frameworks and addressing challenges such as the scalability of large models. Second, it seeks to deepen our understanding of online social interactions through two main approaches: (i) incorporating group interactions and modeling them via hypergraphs and (ii) leveraging LLMs to account for the semantics of these interactions. This multifaceted approach aims to advance our understanding of various real-world phenomena, particularly in social dynamics, as outlined in the research questions in Section 3. By doing so, this project aspires to foster novel insights in a more than-ever interdisciplinary world.

The remainder of this paper is organized as follows. Section 2 describes related works, delineating the gap in the existing literature that motivates my research project. Section 3 outlines the main goals of my research project, the preliminary results achieved, and the challenges I am facing. Finally, Section 4 summarizes the work and indicates the next steps of the project.

2 Background and Related Work

This section provides an overview of how complex systems have been explored in the literature through the lenses of ABM and hypergraphs. It also briefly explains LLMs and discusses their capabilities.

2.1 ABMs

Among the techniques used to analyze real-world systems, ABMs are one of the most effective [6]. From modeling an epidemic spread to an economic fluctuation of the market, ABMs have been used to develop an accurate representation of reality [16, 11]. The main element of an ABM is an *agent*, a basic autonomous entity that the modeler can define with different characteristics and behaviors. Agents can interact with each other and the environment according to a set of rules defined by the modeler. These interactions result in a model of the world being studied, which the modeler can analyze to learn relevant lessons from its emerging behaviors. Structures, patterns, and behaviors emerge through interactions rather than being purposefully coded within the model. ABMs also help researchers determine how a system's micro-level properties, constraints, and laws affect its macroscopic behavior. An agent-based simulation is composed of a three-component structure:

– *Agents.* Each agent is an individual that forms the population under consideration. Agents may act independently or in relation to one another, executing complex functions through simple interactions.
– *Relationships.* The relationships define how agents interact with each other.
– *Rules.* Rules define the agents' behavior, determining the outcomes of their interactions.

Using ABM simulations makes analyzing complex models easier, decomposing the problem into smaller components. However, their implementation can be difficult for domain experts with little experience in software development [1]. The solution to this type of problem lies in multiple frameworks that make it easy to develop and execute a simulation, eliminating the need to know all the necessary technical details. Specifically, simulations have various aspects in common to implement, and these frameworks provide functionality effectively circumventing the need to reinvent solutions for well-known challenges. Good examples of successful ABM engines are Mason, a fast, modular, discrete event multi-agent simulation toolkit written in Java [29], and Netlogo, designed to be used by researchers and educators through a simple interface and language [36].

ABM simulations can be time-consuming because of their particularly high computational load. In addition, their execution time can significantly affect the final result since some simulations achieve greater accuracy as time progresses, as in weather forecasting models. The distributed computing paradigm alleviates such a problem by reducing the running time of long-running simulations without impacting the final outcomes [13]. While, on the one hand, distributed engines have many advantages, on the other, managing the communication and workload between the different machines requires additional effort. In a distributed environment, agents may be simulated on different machines at each time step, thus meaning that the workload should be dynamically adjusted during the simulation. These operations add communication overhead, which adds up to the synchronization step. Further, the whole computation proceeds at the pace of the slowest computer, which could be a barrier to the system's total performance. Another unresolved issue in this context pertains to the reliability of distributed processes, meaning that one should expect functions to either complete successfully or terminate with errors without losing information, even though this may not always be theoretically possible [21]. Frameworks like Mason already provide algorithms and tools to assist their users in implementing distributed ABMs. This design choice allows them to focus only on the simulation-related details without directly dealing with the technicalities of a distributed computation.

2.2 Hypergraphs

A hypergraph is a generalization of a graph where a hyperedge allows the connection of an arbitrary number of nodes. Formally, a hypergraph is an ordered pair $H = (V, E)$ where V is a set of vertices and E is a set of hyperedges. Each hyperedge is a non-empty subset of vertices; that is, $E \subseteq 2^V \setminus \emptyset$, where 2^V is the power set of V [9]. A simple illustration is shown in Figure 1.

Hypergraphs model the extremely non-linear interactions amongst a collection of three or more nodes, thus accounting for additional information [30]. For instance, hypergraphs can abstract social systems in which people interact in groups of any size. One example is the co-authorship collaboration network, where a hyperedge represents an article and links together the authors who have collaborated on it. Other examples can be found in biology, ecology, and neuroscience [7]. One of the few downsides of the strong expressiveness of hypergraphs is that studying these structures requires specific algorithms due to their complexity [24, 28]. Because of this, hypergraphs have not been utilized as much in past literature as their graph equivalent. The use of hypergraphs has been arising recently as a result of numerous systematic studies showing how converting a hypergraph to a classical graph either results in an information loss that cannot be avoided or generates a significant number of additional nodes and edges that increase the amount of space and time needed for analytic tasks [4].

The literature has often studied an entire graph's topology by observing its substructures, commonly known as motifs. In particular, triangular subgraphs appear to be a powerful signal for identifying high-density communities or local trends within a graph [38]. This concept can be generalized to hypergraphs, where h-motifs describe the connectivity patterns of connected hyperedges [26]. Considering an h-motif involving three hyperedges, it is possible to enumerate 26 instances of these substructures. For example, given a set $E1, E2, E3$ of three connected hyperedges, an h-motif describes its connectivity pattern by the emptiness of the sets shown in Figure 2. This definition can be generalized to an arbitrary number of hyperedges and expanded by including a temporal layer to control the evolution of these structures along time [27].

H-motifs can be used to build a hypergraph's characteristic profile (CP) to distinguish the structural design principles of real-world hypergraphs [26]. The

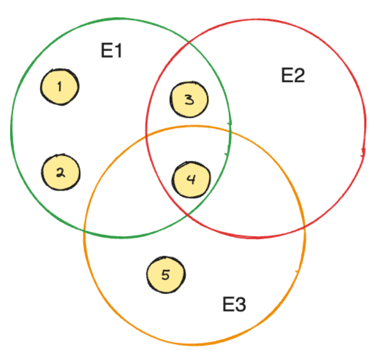


Fig. 1: An example of a hypergraph, with 5 nodes and three hyperedges, E1 = {1,2,3,4}; E2 = {3,4}; E3 = {4,5}.

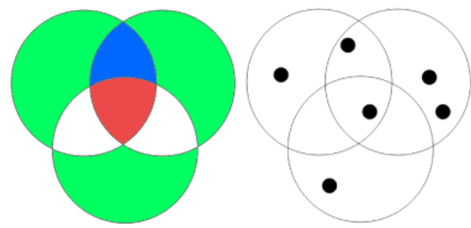


Fig. 2: The image on the left illustrates the intersections between three hyperedges involved in the motif, with colored areas indicating regions of non-empty intersections. The red area represents the complete intersection of three hyperedges; the blue area indicates the intersection of two hyperedges, excluding the third; and the green areas highlight nodes that belong to only one hyperedge. The image on the right depicts a possible instance of this motif.

significance of each h-motif in a hypergraph is measured by comparing the count of its instances against their count in randomized hypergraphs. Specifically, the significance of a h-motif t in a hypergraph H is defined as

$$\Delta_t := \frac{Motif[t] - Motif_{random}[t]}{Motif[t] + Motif_{random}[t] + \epsilon}$$

where ϵ is a parameter fixed to 1 to avoid a possible division by zero when a specific motif does not exist. The CP of a hypergraph H, which summarizes the local structural patterns, is a vector of size 26, where each t-th element is

$$CP_t := \frac{\Delta_t}{\sqrt{\sum_{t=1}^{n=26} \Delta_t^2}}$$

The information conveyed by h-motifs can be leveraged for tasks like hyperedge prediction. According to Lee et al. [26], different motifs produce varying results in this task, possibly because different motifs hold varying levels of importance in different application domains. This finding suggests that further efforts should focus on exploring how selecting the appropriate motifs across various datasets can provide the most valuable insights for the task at hand.

2.3 LLMs

Language models are artificial intelligence models designed to understand, generate, and manipulate human language [20]. These models are used in various applications, such as text generation, translation, and sentiment analysis, to name a few. Language models with hundreds of billions (or more) of parameters, known as large language models (LLMs), are trained on enormous amounts of text data. As an example, we can include GPT [19], LLaMA [37], and Gemma [35]. LLMs generally try to forecast the likelihood of future (or absent) tokens by modeling the generative likelihood of word sequences [40]. These models have been evolving rapidly, from basic language model interfaces to problem-solving agents, demonstrating strong abilities to comprehend natural language and complete challenging tasks via text generation.

Prompting has emerged as the most popular method for using LLMs for various tasks based on the natural language interface. Context learning imbues LLMs with the capacity to perform well on unknown tasks, sometimes surpassing fine-tuned models, by merging task descriptions and demonstration examples into prompts. Advanced prompting approaches, such as the chain-of-thought strategy that incorporates the intermediate reasoning steps into prompts, have been proposed to improve the ability to use complicated reasoning. LLMs enable the development of more intelligent systems (e.g., autonomous AI agents) to tackle various complex tasks in real-world scenarios. With the industry's most recent developments, these tools have many applications, and new ones are found daily [23]. In my PhD project, I leverage LLMs to tackle a stance detection task. Specifically, this task combines hypergraphs for abstracting conversational networks with the analytical power of LLMs to examine their dynamics.

3 Scope

This section details my project's objectives, the research outcomes, and the challenges to tackle across all project topics.

3.1 Project Objectives

The primary objective of my PhD project is to investigate and analyze complex systems by leveraging ABMs, hypergraph-based network models, and LLMs. The specific goals for each of these research areas are outlined below.

ABMs. In the context of ABMs, my goal is to enhance their functionalities to advance the state of the art in ABM engines, particularly regarding their computational limits, as the most widely used ABMs prioritize either performance or usability. Hence, a primary focus of my research is to develop an approach that effectively integrates both features. The main research question my project aims to answer is:

> *How can advances in parallel and distributed computing technologies be harnessed to improve the scalability and efficiency of ABMs for simulating large-scale, real-time, and highly dynamic systems?*

Answering such a question implies validating the following hypotheses:

- H^1_{ABM}**:** Feasibility of developing an efficient and reliable distributed ABM engine.

- H^2_{ABM}**:** Addressing the potential increase in model development complexity through a comprehensive study of system usability from a user perspective.

Hypergraphs. Another main line of work of my PhD project is analyzing group interactions and the rise of collective behaviors in online social media through the lenses of hypergraphs. In this regard, the main research questions my project aims to answer are:

> *Are specific structural patterns in hypergraphs dependent on the communities involved, or do they highlight specific user behaviors? Can we predict the formation of these patterns?*

Answering this question leaves room for several hypotheses, such as:

- H^1_{HG}**:**When analyzing data from the same domain (e.g., conversations about general purpose vs. conversations on domain-specific programming languages), users' activity patterns should differ.
- H^2_{HG}**:** Tracking users across communities and observing their influence can reveal a correlation between structural patterns and specific user behaviors.
- H^3_{HG}**:** When a community of the same users persists over time, its structural pattern should remain consistent.

LLMs. Regarding LLMs, my project's goal is to assess the feasibility of using these tools to extract meaningful insights from text and enhance our understanding of how user interact and exchange their opinions in online social contexts. Specifically, the main research question my project aims to answer is:

> *Can LLMs improve our understanding of online social interactions and opinion dynamics?*

Answering this question leaves space for different hypotheses, such as:

- H^1_{LLM}**:** An LLM can serve as a viable ground truth generator in the absence of annotated conversational datasets.
- H^2_{LLM}**:** Extracting information from text and structures using LLMs can enhance the performance of existing models.
- H^3_{LLM}**:** For stance identification tasks, incorporating high-order interactions that capture the subtle local context of conversations can improve model performance.

3.2 Results

This section presents an overview of the preliminary results achieved during my PhD research. All findings are discussed in relation to the objectives and hypotheses outlined in Section 3.1.

ABMs. As discussed in Section 2.1, over the past decade, the demand for more complex, computation-intensive models has led to the development of numerous frameworks and tools for running ABM simulations. To offer a tool integrating reliability, performance, and ease of use, we developed krABMaga [1, 3], an ABM simulation engine written in Rust. A high-level representation of the architecture of krABMaga is shown in Figure 3.

One of the main goals of krABMaga is to make large-scale simulation available without expensive equipment while still offering efficiency and reliability [3]. Leveraging the Rust programming language has been instrumental in achieving this objective thanks to its performance akin to C, enabled by its memory model, and its expressiveness and usability typical of high-level languages like Python [22]. To further support distributed computation, we developed a custom implementation of a K-Dimensional (K-D) Tree data structure to partition the simulation field and distribute the workload evenly across processes. Unlike traditional K-D Trees, which maintain references to each child in the parent node, our modified approach ensures that all nodes retain references to one another throughout the tree. This adaptation simplifies neighbor search and synchronization operations, crucial for KrABMaga simulations.

Figure 4 shows the performance of our framework running the Flocker simulation, commonly known as Boids [33], on a Microsoft Azure cluster with 128 nodes using the K-D Tree. Specifically, Figure 4a highlights the execution times for simulations with varying numbers of agents (1M, 2M, 5M, and 10M), while Figure 4b showcases the speedup achieved in each experiment. This second plot reveals an increased speedup as the number of agents grows, attributed to the effective management of agents by the simulation processes. This efficiency becomes more pronounced when the computational workload exceeds the communication overhead. The results closely follow the ideal performance curve, where speedup scales linearly with the number of processors or machines (e.g., 2 processors yield a speedup of 2, 4 processors yield a speedup of 4, etc.). In future work, we aim to develop a more robust communication layer that is entirely transpar-

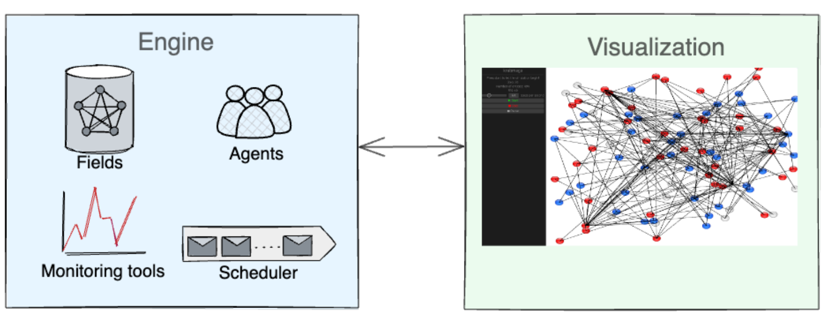
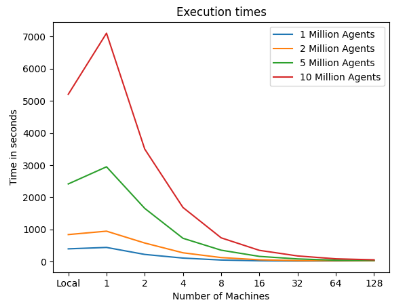
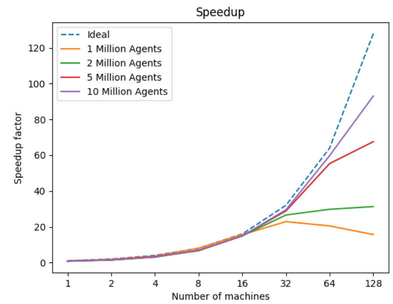


Fig. 3: A high-level illustration of the architecture of krABMaga: the Engine module includes the core functionalities of the framework (on the left), while the Visualization module orchestrates visualization-related features (on the right).



(a) Execution times.



(b) Relative speedup.

Fig. 4: Performance of krABMaga in a distributed environment (Microsoft Azure cluster with 128 nodes) during simulations of the Flocker model with a growing number of agents.

ent to the modeler to further simplify the simulation process by removing the need to implement complex custom functions.

Currently, we are working on integrating Geographic Information System (GIS) data into our engine. As illustrated in Figure 5, we implemented a plugin that allows users to upload a file containing a map (e.g., the US territories) and convert it into one of the krABMaga fields, enabling agents to move on top of it. In this manner, krABMaga will empower users to simulate more diverse and realistic scenarios.

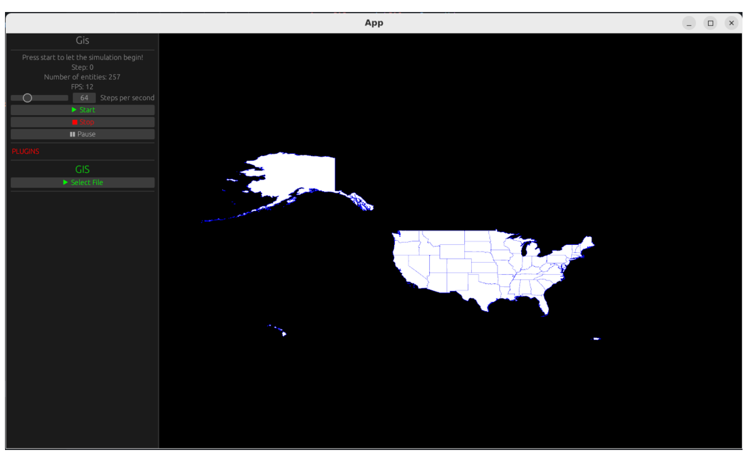


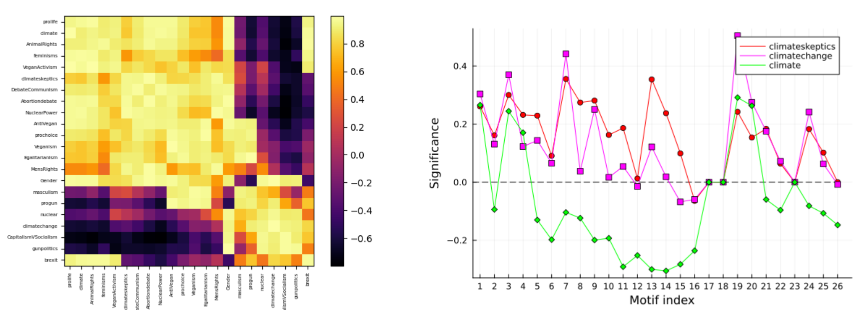
Fig. 5: Graphical user interface of krABMaga, demonstrating the implementation of the GIS plugin.

Hypergraphs. Online social networks generate vast amounts of data. Websites like Facebook, YouTube, or Reddit have millions or billions of users that interact daily. My focus in this context is analyzing group interactions and the structural and semantics patterns of user communities in online social media through the lenses of hypergraphs.

In a first study, we analyzed developers' behavior and the formation of communities around twenty popular programming languages, emphasizing the significant differences in how users engage in different Question & Answer (Q&A) platforms, such as StackOverflow and Reddit [2]. Q&A platforms, and social networks in general, usually consist of discussions in which users reply to each other on the same topic. Hence, conversational networks provide opportunities to identify strongly connected communities and examine whether specific user behavior depends upon the characteristics of the given platform. Looking at the CP of such conversations could give deeper insights into user communication patterns and their similarities across topics, communities, and platforms. Figure 6a shows the CP of 22 different subreddits as an example of this analysis. Preliminary results indicate that conversations on similar topics do not necessarily exhibit similar CPs. This observation is further confirmed in Figure 6b, showing the CPs of three subreddits related to climate change.

Unfortunately, access to the API or raw data of many online social platforms is often limited or behind a paywall, posing a barrier for researchers interested in studying online behaviors. As a consequence, having a ready-to-use dataset to carry on specific analyses is not always trivial. To alleviate such a problem, we published an open-source online repository to allow researchers to compare and download data tailored for high-order analysis [5].

LLMs. Another interesting line of inquiry that has emerged recently is the use of LLMs to gain insights into both structural and linguistic attributes of



(a) Similarity matrix of CPs of 22 subreddits on different topics.

(b) CPs of 3 climate-related subreddits.

Fig. 6: CP-based similarity across different subreddits.

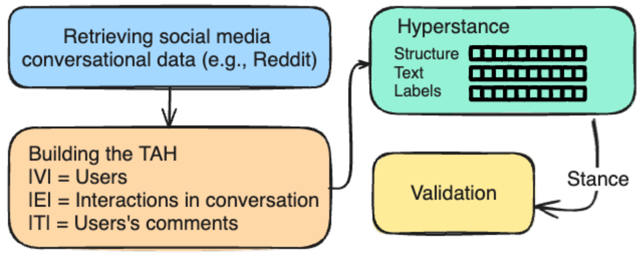


Fig. 7: A proof-of-concept pipeline to investigate a machine learning model combining semantics and structure.

conversational networks. The architecture depicted in Figure 7 represents our initial attempt to combine hypergraphs (to learn the conversational hypernetwork's structure) and LLMs (to understand the text's semantics) for performing a stance detection task [17]. Specifically, stance detection involves automatically classifying a user's attitude toward a target into one of three categories: *Favor, Against, Neither*.

In our experiments, we focused on the Reddit discussion platform, selecting three subreddits centered around the climate topic (i.e., *climate, climatechange, climateskeptics*), and retrieved all users' conversations over a two-year period. To obtain an initial training set, we used Gemma [35], a recently published LLM, to label a real-world dataset from Reddit, annotating the stance of all the messages, while the results obtained will be validated against a social network dataset annotated by humans for the same task [34].

3.3 Challenges

These topics come with many theoretical and practical challenges to consider.

ABMs. Regarding ABM, there are two main problems to deal with. First, ABMs can be computationally intensive, especially when simulating large numbers of agents or complex interactions between agents [31]. This can limit the scale and scope of simulations that can be conducted, particularly on basic computing hardware (e.g., personal laptops). Furthermore, ABMs often require significant parameterization and calibration to represent real-world systems accurately. Identifying appropriate parameter values and validating the model against real-world data can be challenging and may introduce uncertainties in the model [32].

Hypergraphs. Hypergraphs are a growing field, but there is a lack of standardization regarding definitions, models, and algorithms. Due to the arbitrary size of the relationships between nodes, dealing with hypergraphs implies interacting with a more complex network than a traditional graph. One example of this increased complexity is the visual representation of hypergraphs, which is often depicted using Venn diagrams. However, drawing such representations becomes nearly impossible or extremely chaotic as the number of nodes and hyperedges grows. While graphs can be easily represented with points and lines, hypergraphs require circles or other techniques that do not always provide intuitive insights, necessitating the introduction of valid alternatives [18].

Another challenging task on hypergraphs is link prediction. In a graph, link prediction involves predicting the existence of a specific relationship between two nodes. This definition does not translate well to hypergraphs, where a hyperedge may include an arbitrary number of nodes [4]. In this context, predicting the appearance of an h-motif is even more challenging, as it requires understanding not only if a link will connect certain nodes but also if it will form a specific substructure with other existing links.

LLMs. Although LLMs offer numerous advantages, they also present several drawbacks. One of the most notable issues is bias. Training LLMs on massive datasets can inadvertently reinforce preexisting inequities or omit important perspectives due to biases in the data. Moreover, LLMs are often seen as black box models, making it difficult to understand how they reach their conclusions. This lack of interpretability can hinder trust and acceptance of their analyses, especially in scientific contexts where transparency and reproducibility are crucial. Finally, LLMs may struggle with understanding the context of a task, particularly in specialized domains where terminology and conventions vary significantly. Misinterpreting context can lead to inaccurate analyses.

4 Conclusion and Future Work

Studying social systems encompasses a variety of open problems, ranging from examining emergent behaviors to algorithmically analyzing how to prevent the spread of misinformation. My PhD project aims to enhance our understanding of social dynamics in online social media by considering group (or high-order) interactions and to provide tools for easily and efficiently studying human dynamics. Specifically, the current contributions of my PhD research can be summarized as follows:

- **ABMs.** We (i) conducted an in-depth review of existing ABM tools to identify current trends, challenges, and opportunities for innovation; (ii) developed a stable version of krABMaga, an ABM simulation engine, and various simulation models (contributing to H^1_{ABM}); (iii) extended the features and capabilities of krABMaga to include distributed computation and GIS data integration. Additionally, we focused on enhancing the system's usability by creating an easy-to-use GUI (addressing H^2_{ABM}).
- **Hypergraphs.** We (i) developed a community-driven open-source platform to store hypergraph datasets; (ii) examined interactions in online social media groups through the lenses of hypergraphs (contributing to H^1_{HG}); (iii) investigated the application of modern techniques, such as graph neural networks, to analyze high-order interactions (contributing to H^2_{HG}).

- **LLMs.** We (i) analyzed the semantic information within the text linked to each node in a hypergraph using LLMs (contributing to H^1_{LLM}); (ii) developed a model to embed LLM-generated information into a stance detection task (addressing H^2_{LLM}).

In future development, we aim to: (i) continue developing new simulation models, conducting performance benchmarks, and adding features and plugins (e.g., other distributed fields, visualization functionalities) to krABMaga; (ii) thoroughly explore the influence of patterns on opinion change within conversational data; (ii) explore how LLMs can be utilized to enhance our understanding of text in online social contexts.

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