

MATHVC: An LLM-Simulated Multi-Character Virtual Classroom for Mathematics Education

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Abstract

Mathematical modeling (MM) is considered a fundamental skill for students in STEM disciplines. Practicing the MM skill is often the most effective when students can engage in group discussion and collaborative problem-solving. However, due to unevenly distributed teachers and educational resources needed to monitor such group activities, students do not always receive equal opportunities for this practice. Excitingly, large language models (LLMs) have recently demonstrated strong capability in both modeling mathematical problems (Wei et al., 2022) and simulating characters with different traits and properties (Park et al., 2023). Drawing inspiration from the advancement of LLMs, in this work, we present MATHVC, the very first LLM-powered virtual classroom containing multiple LLM-simulated student characters, with whom a human student can practice their MM skill. To encourage each LLM character’s behaviors to be aligned with their specified math-relevant properties (termed “*characteristics alignment*”) and the overall conversational procedure to be close to an authentic student MM discussion (termed “*conversational procedural alignment*”), we proposed three innovations: integrating *MM domain knowledge* into the simulation, defining *symbolic schema* as the ground for character simulation, and designing a *meta planner* at the platform level to drive the conversational procedure. Through experiments and ablation studies, we confirmed the effectiveness of our simulation approach and showed the promise for MATHVC to benefit real-life students in the future.¹

1 Introduction

Mathematical modeling (MM), the process of creating a mathematical representation of a real-world problem, is a critical skill for students pursuing STEM fields. Practicing this skill often requires students to engage in effective discussions of relevant concepts and collaboratively solve mathematics problems with their classmates (Vygotsky & Cole, 1978; Garfunkel & Montgomery, 2019). However, orchestrating such discussions and collaborative learning activities can be very challenging for teachers (Bush et al., 2020). As a consequence, the Opportunity Myth report (TNTP, 2018) has highlighted that students from marginalized communities where only limited teachers and educational resources are available, are less likely to have opportunities to participate in effective practices of MM skills.

The rapidly developing large language models (LLMs) have shown huge potential to reshape the future of education (including Mathematics) (Denny et al., 2024). This potential stems from two recent advancements uniquely for LLMs. Firstly, LLMs present strong math reasoning capabilities in understanding and solving mathematics problems (Wei et al., 2022; Lu et al., 2023; Ahn et al., 2024). In particular, on the GSM8k dataset (Cobbe et al., 2021) representing middle-school mathematics level, the state-of-the-art GPT-4 model has

¹Source code and examples will be available at our project website soon.

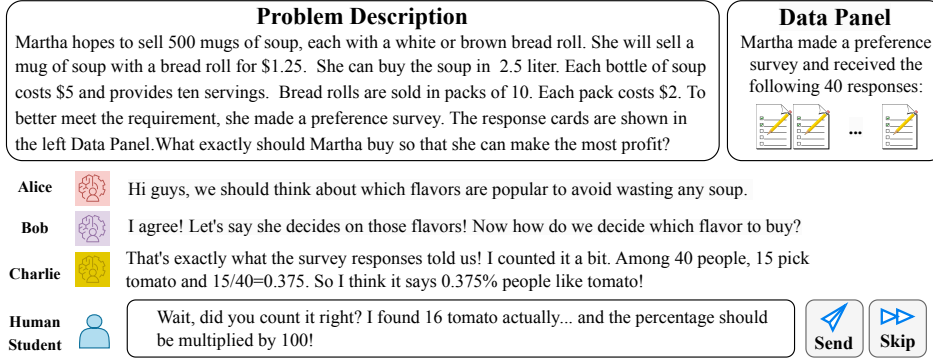


Figure 1: An example demonstrating the application of MATHVC, where students are presented a math problem (optionally with accompanied data) and engage in effective discussions on math modeling. Alice, Bob, and Charlie² are LLM-simulated student characters. A human student can choose to respond or skip the current turn.

achieved close to perfect performance (OpenAI et al., 2024). Secondly, by generating human-like thoughts and actions in explicit texts, autonomous LLM-based generative agents have showcased the capacity to simulate human activities (Park et al., 2023; Wang et al., 2023c; Zhou et al., 2023). Leveraging this capability, studies have explored simulating human behaviors in different scenarios, such as games (Wang et al., 2023a), social activities (Li et al., 2023b; Cheng & Chin, 2024), software engineering (Hong et al., 2023; Qian et al., 2023).

Observing the pressing need to enhance MM education for resource-limited communities and getting inspired by the striking progress made by LLMs, in this work, we propose **MATHVC, a Mathematics Virtual Classroom** (Figure 1) featuring multiple LLM-simulated student characters, with whom a human student can discuss and collaboratively solve MM problems, which thus allows them to practice their MM skills without needing the teachers monitoring it. In particular, the platform focused on *middle-school* MM problems, a difficulty level that has been well handled by GPT-4. To the best of our knowledge, our research is the *first* work exploring the potential of leveraging LLMs and LLM-powered generative agents for mathematics education. We envision that such a platform can eventually be deployed as part of the middle-school curriculum, enabling effective MM learning to go beyond the space constraint in traditional classroom studies while enhancing students’ MM capability.

We identified two unique challenges in the development of MATHVC. The first challenge is **characteristic alignment**, i.e., *aligning an LLM’s character simulation to the authentic characteristics of real human students*. Middle-school students in real life could struggle with rapid and accurate modeling. They may initially produce incomplete or erroneous mathematical models and refine them iteratively as the discussion progresses. This process of gradually establishing mutual understanding with teammates, interleaved by continual self-reflection, is the key for students to improve their MM skills. However, in our preliminary experiments using GPT-4, a vanilla character simulation via prompt engineering the profile instruction to LLM cannot yield such an authentic and fine-grained student simulation. Instead, GPT-4 often directly gives a close-to-perfect solution, even when prompted to simulate students with poor math skills. Simulating how a student’s problem understanding and math modeling evolve during the collaboration, is even more difficult. The second challenge is **conversational procedural alignment**, i.e., *aligning the overall conversational procedure to an authentic MM discussion among middle-school students*. While the first challenge concerns individual characters’ simulation, this second challenge considers inter-character interaction. In practice, a collaborative problem-solving process typically consists of multiple stages, including problem understanding, task division, solution planning, plan execution, etc. (PISA, 2018). However, when we directly exposed the group of LLM characters to interact with each other, these LLM characters often bypassed the earlier stages and instead, initiated the conversation by immediately describing a modeling solution. For both of the two

²We use the three names as “placeholders” following the convention in science and engineering literature (Wikipedia, n.d.); however, we envision the system to be used by various communities.

challenges, we conjecture that the vanilla simulation fails because LLMs were pre-trained in a question-answering style (e.g., they tend to directly give answers to the input mathematics questions), while lacking sufficient *instructibility* to follow the prompt instruction and simulate the deliberation of a middle-school student. Despite existing exploration of LLM character simulations, we have not seen any prior work carefully exploring these two alignment challenges and the solutions to them.

To tackle these challenges, we propose to integrate relevant theories of MM and collaborative problem-solving (CPS) (Standards, 2010; PISA, 2018) into the development of MATHVC. Specifically, to enhance characteristics alignment, we propose using a symbolic *character schema* to represent the *dynamic* problem understanding process of a character. The character schema centers around “variables” that are essential for solving the mathematics problem, which are considered fundamental elements in MM theory (Standards, 2010). By considering it as a “ground”, we can simulate characters with more intricate behaviors, including how they make a mistake initially and then gradually fix it during the collaboration with other students. To enhance conversational procedural alignment, we further propose a *meta planner* at the platform level, which monitors the overall conversation and plans its procedure following the stages defined in the CPS theory (PISA, 2018).

Through experiments and ablation studies, we confirmed the effectiveness of our simulation. Specifically, we compared MATHVC with vanilla character simulation as well as its variants when it is augmented with math theories in prompt formulation or is equipped with our proposed character schema and meta planner. The results showed that MATHVC can achieve the best performance for simulating both individual characters and character interaction. Overall, our generated multi-character dialogues can better reflect the predefined student characteristics and are more akin to conversations among real middle-school students in collaborative MM tasks. We also conducted a series of ablation studies for two key components in MATHVC (i.e., meta planner and the character schema); the results validated the necessity of our proposed prompt designs. In summary, our results indicate that MATHVC has huge potential for being deployed to serve middle-school students in real life, and our proposed approaches can be generalized to resolve similar alignment problems in other applications.

2 MATHVC: An LLM-Powered Mathematics Virtual Classroom

2.1 Overview

Our goal is to develop a “virtual classroom” platform with multiple LLM-simulated student characters discussing and collaboratively solving MM tasks. We propose to design MATHVC with a modular architecture as shown in Figure 3. Specifically, the system consists of two parts, i.e., **meta planner** for organizing the overall conversation and facilitating a smooth multi-stage student discussion, and **character simulation** for creating and updating individual student characters. All modules in MATHVC are implemented by prompting an LLM (e.g., GPT-4) with specialized scripts, mostly in zero-shot (except for Dialogue Act Generator in one-shot). A complete workflow of the system is presented in Appendix A.

2.2 Symbolic Representations for Task and Character Modeling

A key innovation of MATHVC lies in the use of *symbolic schemas* describing how characters form and gradually update their understanding of the mathematics problem. Specifically, we design two schema representations. **Task Schema** is a template describing elements that are necessary for solving a given MM task. As shown in Figure 2 (left), a task schema specifies how the original mathematics problem can be decomposed into multiple sub-tasks, and for each sub-task, what variables should be defined to resolve it. In other words, a task schema shows the ground-truth understanding and modeling of a mathematics problem. We define the schema centering around “variables” because they are considered the fundamental elements in MM (Standards, 2010). In practice, this schema can be automatically generated by prompting an LLM with the mathematics question and the ground-truth step-by-step solution following the Chain-of-Thought (Wei et al., 2022, CoT) formulation. Note that while a task schema could be challenging and time-consuming to manually annotate for teachers using this platform, the step-by-step solution is easy to compose or can be scraped from the answer notes of textbook exercises or directly generated by GPT-4.

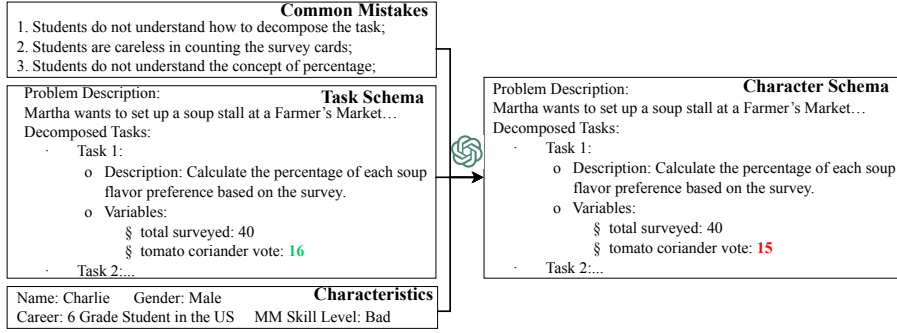


Figure 2: Example task and character schema. The LLM edits the correct value **16** into **15** in the task schema to simulate the initial mistake made by the simulated student Charlie.

Built on top of the task schema, we further devise **Character Schema**, a symbolic representation showing a student character’s understanding and modeling plan on the given mathematics problem. As shown in Figure 2 (right), a character schema is a task schema injected with errors that could be made by real human students. We consider a wide range of errors including misunderstanding on a sub-task or even omitting the sub-task, as well as any variable mistakes resulting from miscounting, incorrect modeling, or calculation errors. In mathematics education, materials such as the lecture notes in the Mathematics Assessment Project (MAP) (MAP, n.d.), often summarize common mistakes in each math problem, which can be directly used for simulating how students had incorrect solutions in the beginning. In MATHVC, the character schema is synthesized by prompting an LLM to *edit* a task schema based on the student’s characteristics as well as a set of possible mistakes. Throughout the conversation with other students, a character will gradually update its character schema to reflect its dynamic thought process, as we will introduce in Section 2.4.

2.3 Meta Planning

The main goal of the meta-planning module is to perform meta-level control of the entire conversation to encourage conversational procedural alignment. It consists of three components: (1) **Task Schema Generator**: As Section 2.2 mentioned, the initial step of MATHVC is to generate the task schema, which can then be edited to form character schemas. We instruct the LLM to produce the task schema with the specified format shown in Figure 2. A rule-based text checker will be applied to verify if the generated schema follows the format; if not, we regenerate a new one. (2) **Collaboration Stage Monitor**: Prior work (PISA, 2018) has observed that the collaborative problem-solving (CPS) process among students often consists of a sequence of stages, such as first establishing a shared task understanding and then establishing a team organization, as we summarize in Figure 3 and explained in Appendix B. To ensure that our simulated discussions closely resemble real CPS discussions, every dialogue will start from Stage 1, with the collaboration stage monitor dynamically determining whether the current stage is completed and whether the discussion should proceed to the next stage. This decision is made based on the dialogue history as well as a definition of every stage. When all stages are completed, we end the session. We note that simulating this multi-stage process is also important for human students to engage in effective MM practices, as it enables more *scaffolded* human and character interaction. (3) **Dialogue Speaker Control**: To facilitate smoother conversation interactions, we have developed a dialogue speaker control module that predicts the next speaker based on the dialogue context. For instance, if the last response is “Hey Bob, you made a mistake...”, the next speaker is likely Bob. The LLM captures this intuition by learning from the dialogue history, and it is prompted to output a single character name as the next speaker.

2.4 Character Simulation

Each character is simulated with four specified traits: name, gender, career (e.g., grade level in our application), and MM skill level (i.e., good or bad³). We included the first two traits

³In this work, we define a student’s MM skill in a coarse way. Future work could enhance it to be more fine-grained based on the practices in mathematics education.

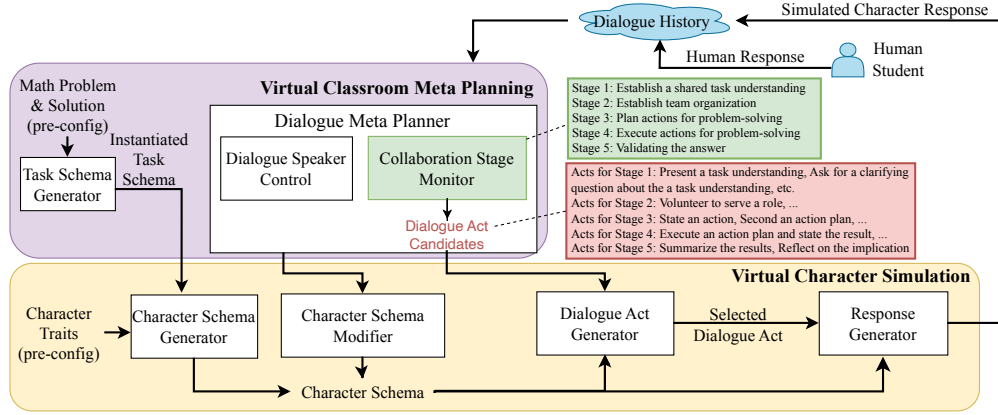


Figure 3: Architecture of MATHVC for simulating student characters and multi-character conversations in collaborative MM problem-solving.

mainly for characters to address each other (via names or pronouns) and the last two for configuring each character’s MM background.

Our simulation functions with four components (Figure 3, bottom). The first two components are responsible for generating and maintaining the character schema. (1) **Character Schema Generator**: As we introduced in Section 2.2, every simulated student character has its own character schema to reflect their thought. In our simulation, a character schema generator decides the specific mistake(s) a student character will make based on their traits and then edits the task schema into their initial character schema (Figure 2). To facilitate this editing, as shown in Appendix C, we represent the task schema as a Python dictionary and express every edit as a line of Python code that specifies the replacement of a variable or a sub-task description. (2) **Character Schema Modifier**: During real-life student discussions, a human student’s thought for a given question often evolves as the conversation progresses. We simulate these dynamics by continuously modifying the character schema based on the dialogue history. We prompt the LLM to decide whether the current schema needs to be modified. When it does, the modification will be achieved by generating a Python code that edits the previous character schema, similar to the initial character schema generation.

Generating character responses is not a trivial task in our application. A major challenge we observed is their *lack of diversity*. For example, when we directly prompted LLMs to generate responses simulating how students discuss their modeling plans (i.e., Stage 3), all responses were uniformly assertive statements of a plan, without other forms of communication that are also commonly seen in authentic student discussions (e.g., question-answering). To address the issue, we propose a two-step response generation with the following two components. (3) **Dialogue Act Generator**: Before the response generation, we first prompt the LLM character to pick a “dialogue act” indicating the intent of their response. Dialogue acts are widely used in traditional dialogue systems (Stolcke et al., 2000; Li et al., 2016; Zhao et al., 2017). In our application, we define a set of dialogue acts for each conversational stage, such as “present a task understanding” and “ask for a clarifying question about a task understanding” for Stage 1, as shown in Figure 3; the complete definitions can be found in Appendix B. A dialogue act generator is then tasked to *generate* a dialogue act (e.g., “ask Bob a clarifying question about...”) based on the character schema, the dialogue history, and the set of dialogue acts for the current stage. We found that the use of dialogue acts could dramatically increase the response diversity when an LLM is explicitly prompted to reason about the proper response (e.g., asking a clarifying question when the character has a different modeling plan than their teammates, or generating a narrative answer when a character is asked for clarification). (4) **Character Response Generator**: Once deciding the dialogue act, a character response can be generated conditionally. However, even when the character schema is provided in the prompt, we still observe inconsistency between the character schema and the generated response (e.g., characters referring to inconsistent variable values than those in their schemas). To make the response follow the character schema better, instead of directly generating, we prompt an LLM to first retrieve relevant

System	Characteristic Alignment	Conversational Procedural Alignment
Vanilla Simulation	2.85	2.88
Domain-Specified Simulation	3.30	3.15
w/ only character schema	3.50	3.20
w/ only meta planner	3.00	3.10
MATHVC	3.73	3.53

Table 1: Human evaluation results comparing various simulations (1: worst; 4: best).

variables from the character schema, and then generate a response conditionally on the variables and their values. In practice, we found this prompt design to be very effective. Additionally, in the prompt, we instruct the LLM to mimic the language style of middle-school students (e.g., keeping the response short and colloquial). We present the prompts for the dialogue act generator and the response generator in Appendix I.

3 Experiment

3.1 Experimental Setup

Dataset and Experimental Setting We conducted experiments using middle-school mathematics problems from the MAP project (MAP, n.d.) and GSM8k (Cobbe et al., 2021). Questions from the MAP include both answers and common student mistakes, while those from the GSM8k only have answers; therefore, we manually annotate mistakes for them.

The most ideal evaluation of MATHVC is to include real middle-school students in the loop, but this is very challenging and unsafe to implement (see our Ethics Statement). As our purpose of this work is mainly to showcase the feasibility of such a virtual classroom, during evaluation, we exclude real-student interaction and only focus on whether the multiple (3 in our experiments) simulated LLM characters can reasonably collaborate on solving MM tasks. The evaluation is then conducted by sampling multiple simulated dialogues and manually assessing their quality. Due to the cost of manual evaluation, we sample a small set of questions (5 as the dev set and 10 as the test set). For each question on the test set, we consider two student character configurations with varying MM skill combinations, and sample one multi-character dialogue in each for every system in comparison. We used GPT-4-turbo as the backbone LLM. We include more experimental details in Appendix D.

Baseline Systems We compare MATHVC with four baselines. (1) **Vanilla Simulation** follows the prior work (Park et al., 2023) in prompt engineering the profile instruction to an LLM. Specifically, we directly present the LLM the math question, the student characteristics, and the dialogue history, and then instruct the LLM to generate responses as a middle-school student. (2) **Domain-Specified Simulation** further augments the vanilla simulation with domain-specific knowledge in its prompt, including the stages and possible acts in each stage, common student mistakes, the language style of a middle-school student, and so on. To demonstrate the effectiveness of our character schema and the meta planner, we include two more variants on top of domain-specified simulation, i.e., **(2.1) w/ only character schema**, where we include our proposed character schema in the prompt to the LLM and allow for continual schema modification, and **(2.2) w/ only meta planner**, where we augment the domain-specified simulation with our meta planner. The planned stage is added to the prompt for character response generation.

Evaluation Metrics The human evaluation was conducted by two student annotators. The annotators were instructed to rate each sampled dialogue on the degrees of characteristic alignment and conversational procedural alignment it reflected (1: worst; 4: best). We report an average score. More details and the annotation guideline are presented in Appendix H.

3.2 Experimental Results

The human evaluation results are shown in the Table 1. We make the following observations:

Incorporating domain knowledge improves the simulation quality. All systems built with domain knowledge outperform the vanilla simulation. In our inspection, we observed that the vanilla simulation cannot simulate fine-grained student behaviors; for example, it rarely exhibits modeling mistakes even when simulating students with bad MM skills and

often starts the discussion unnaturally with solution statements. By introducing knowledge of common mistakes and stage information to its prompt, these issues are mitigated in domain-specified simulation, leading to improved alignment on both characteristics and conversational procedures.

Including character schema enhances characteristic alignment, but including meta planner enhances alignment only when used with character schema. Incorporating solely character schema could improve the characteristic alignment and result in comparable conversational procedures. Surprisingly, we observe that simply adding the meta planner may even degrade the dialogue quality. We found that when adding the natural-language stage information (e.g., “*execute actions for problem-solving*”) explicitly to the prompt of domain-specified simulation, the LLM was biased to respond with a direct solution (e.g., presenting the execution results). This not only broke the characteristics but also resulted in unnaturally shorter conversations. The observation, on the other hand, confirms the necessity of the dialogue act generator of MATHVC, which avoids this issue by inferring the likely dialogue acts in each stage and feeding the dialogue acts rather than the explicit stage information for response generation.

MATHVC offers the most aligned simulation by harmoniously integrating character schema with meta planner. Our system obtained the highest scores on both alignment aspects, demonstrating the effectiveness of integrating the symbolic schema representations with meta-planning under our framework. We qualitatively compare MATHVC with other approaches in Figure 4. In the vanilla simulation, the discussion bypasses many discussion stages (e.g., establishing the team organization), and Alice, who is bad at mathematics, does not make any mistakes. The domain-specified simulation made some improvements, such as simulating responses that are shorter and can simulate how students establish shared task understanding before planning on problem-solving, although it is still unable to simulate a fully extended, multi-stage conversation (e.g., team organization is still missing). In MATHVC, the conversation successfully goes over all stages. It also simulates how Alice makes a calculation mistake initially, which is then corrected by Charlie. Like a real student, Alice then adjusts her modeling plan based on Charlie’s explanation. This case study demonstrates the superiority of our system in both the characteristics alignment and the conversational procedural alignment.

3.3 Further Analysis and Discussion

Ablation Studies Evaluating Key Prompt Designs in MATHVC We further conducted ablation studies to validate the key prompt designs in MATHVC, hoping to share insights with future research that will simulate characters at the same complexity level. Our investigation reveals that (1) editing is superior to regenerating in the character schema modifier; (2) generating acts is preferable to solely selecting acts in the dialogue act generator; and (3) two-step generation is more effective than the direct generation in the response generator. The results and analysis are in Appendix E.

Error Analysis Through analyzing the sampled dialogues, we identify two key issues of MATHVC that can be addressed in the future. First, we observed that the LLM-simulated students sometimes cannot elaborate on their deliberation process. Rather, they tend to directly offer an opinion, which makes the conversation less engaging. Second, *instructibility* remains a major challenge in the character simulation. For example, even when a character has been simulated to take charge of a certain sub-task during the team organization, the LLM may still generate a response mistakenly representing the character’s actions in solving a different sub-task. We conjecture that this discrepancy is sourced from the LLM’s attention to dominantly the local context (e.g., the current sub-task focus), while instructions indicated in the relatively distance context are overlooked (e.g., Alice’s sub-task assignment at the beginning of the discussion). Future work could address these issues by designing an appropriate schema to encourage responses with details and dynamically store and retrieve information in both long- and short-term character memory.

Preliminary Results with Humans in the Loop While we are not able to recruit middle-school students in our current research, we conducted a preliminary study showing the potential for real humans to engage in collaborative MM tasks with LLM characters. An example dialogue conducted by one author is shown in Appendix F. We found that the

Problem Description: Steve loves playing video games. His parents get him a console along with 5 games for his birthday. He saves up enough money to buy 1 game per month for a year, and then the following year he starts buying 2 games a month. For the third year he buys 4 games a month as he has a new part-time job that makes him more money. He also gets 5 games for Christmas every year. How many games does Steve have after 3 years?	Character Configuration: Alice: Female, Grade 6, MM: Bad Bob: Male, Grade 6, MM: Good Charlie: Male, Grade 6, MM: Good
<p><i>(Planning & Problem Solving)</i></p> <p>Bob: Hey everyone, so we're trying to figure out how many games Steve has after 3 years, right? Let's break it down year by year. In the first year, he starts with 5 games from his birthday. Then he buys 1 game per month, which means 12 games in a year, right? So at the end of the first year, he has $5 + 12$ games. Plus, he gets 5 more games for Christmas. That's $5 + 12 + 5$. Does that make sense so far?</p> <p>...</p> <p>Alice: Oh, okay, I think I'm following. So for the first year, Steve has 22 games in total. Now, for the second year, Charlie said he gets 24 games because he buys 2 each month, and then another 5 for Christmas, so that's $24 + 5$ for the second year. If we add that to the first year's 22 games, let me think. That's $46 + 5$... which is 51 games at the end of the second year, right? Now, for the third year, he buys 4 games a month, and there are 12 months, so that's 4 times 12... um, I'm not great at math, but I think that's 48 games? Plus, he gets another 5 for Christmas. So for the third year, he has $48 + 5$ games. We need to add that to the 51 games he already has from the first two years. So, $51 + 48 + 5$... that's $99 + 5$... which is 104 games in total after three years.</p>	<p>Vanilla Simulation</p>
<p><i>(Establishing Shared Understanding)</i></p> <p>Alice: Okay, so first we need to figure out how many games Steve gets each year, right?</p> <p>...</p> <p><i>(Planning & Problem Solving)</i></p> <p>Alice: Oh, I almost forgot about the monthly games. So, for the first year, it's 12 from buying one each month, and then 5 for Christmas, right?</p> <p>Bob: Yes, that's 17 games for the first year.</p> <p>...</p> <p>Charlie: But don't forget, we need to add the initial 5 games he got with his console to the total as well. So that would be 104 games after 3 years.</p> <p>Alice: Oh yeah, I missed those first 5 games. So with those, Steve has 104 games in total after 3 years.</p> <p>Bob: Right, so we have 17 games from the first year, 29 from the second year, and 53 from the third year, plus the initial 5 games from his birthday. That makes 104 games in total.</p> <p><i>(Validating the result)</i></p> <p>Charlie: Looks like we've got it all covered. Steve ends up with 104 games after 3 years.</p> <p>Alice: Great, so we all agree that Steve has 104 games after 3 years. Good job, everyone!</p>	<p>Domain-Specified Simulation</p>
<p><i>(Establishing Shared Understanding)</i></p> <p>Alice: Okay, so for our project, we need to calculate the number of games Steve buys each year for three years, the games he receives as gifts for Christmas, and then the total number of games he has after three years.</p> <p>Bob: Got it, Alice. So we'll be tracking Steve's game purchases over three years, his Christmas gifts, and then summing it all up to find out his total game collection after that period. I think we should divide the tasks. Maybe one of us can handle the game purchases, another the Christmas gifts, and a third could work on the total calculation. What do you guys think?</p> <p><i>(Establishing Team Organization)</i></p> <p>Alice: I can take care of calculating the game purchases Steve makes each year. Does anyone want to handle the Christmas gifts, or should we rotate that responsibility?</p> <p>Charlie: I can handle tracking the Christmas gifts Steve receives. We could also set up a shared document to monitor our progress. Does that work for everyone?</p> <p>Alice: Great idea, Charlie! Who would like to take on the total calculation, or shall I add that to my tasks?</p> <p>Charlie: I'm on board with tracking the Christmas gifts. Bob, would you like to handle the total calculations, or should we discuss this further?</p> <p>Bob: I'm happy to handle the total calculations.</p> <p><i>(Planning & Problem Solving)</i></p> <p>Alice: Let's start by figuring out how many games Steve buys in the first year, which is simply the number of games he gets each month times the number of months in a year.</p> <p>...</p> <p>Charlie: So if we add up all the games Steve bought over the three years, which is 12 the first year, 24 the second year, and 48 in the third, plus the 15 games he got for Christmas, he'll have a total of 99 games after three years!</p> <p>Alice: You nailed it! So he has a total of 99 games after three years. Let's double-check the starting number just to be sure!</p> <p>Charlie: Hey Alice, he actually has a total of 104 games!</p> <p>Alice: Can you explain why you think it's 104?</p> <p>Charlie: Actually, Alice, Steve started with 5 games, not zero, so if we add those to the 99 games he got over three years, it's 104 games in total. We should double-check the starting number to make sure we've got it right, and I'll update our shared document with the correct total!</p> <p>Alice: Charlie, you're right, Steve did start with 5 games, and if we add all the games he got over the years, it's 104 games in total!</p> <p><i>(Validating the result)</i></p> <p>Charlie: Yep, I've double-checked, Steve has a grand total of 104 games after three years, including the 5 he started with and all the gifts and purchases!</p> <p>Bob: Awesome, everything checks out! Steve's game collection is definitely at 104 games after three years!</p>	<p>MATHVC (Ours)</p>

Figure 4: Case study for different simulation approaches. We manually annotated the simulated stages in blue and indicated responses reflecting Alice's bad math skill in red. In the vanilla simulation, Alice merely verbally indicates that she struggles with math but still gives a correct calculation "48", whereas in MATHVC, she makes a genuine mathematical modeling mistake.

interaction between the human and the simulated student characters is natural and effective. It showcases the promise for future deployment with real middle-school students.

Simulation with Varying Character Names, Genders, and Careers Our main evaluation has focused on the simulation of students at different MM skill levels, given that it is the most essential demand for MATHVC. To further understand the impact of other traits, we present sampled dialogues with different character names (other than the “placeholders” Alice, Bob, and Charlie), genders (e.g., when all characters are females), and careers (e.g., when characters come from different grade levels or countries). Our ablation analysis as described in Appendix G shows that these characteristics have only a minor impact on the response, and we did not observe any ethical concerns (e.g., biases) in our examination. We include further discussions in the Ethics Statement.

Limitations and Future Work Like most existing LLM agents, MATHVC faces the issues of token costs and latency, when it has to query an LLM multiple times for each character’s response generation. In our early study, we experimented with the relatively cheaper and faster GPT-3.5-turbo but encountered unsatisfactory results. On the other hand, the pipeline design of MATHVC’s architecture could lead to error accumulation, i.e., when one module does not yield satisfying outcomes, the following ones suffer the same. However, overall MATHVC still demonstrated a huge potential to be deployed to serve real students and be used as a tool for mathematics education. In the future, one important extension is to allow for “personalization” of MATHVC, such as simulating student characters based on the specific human student’s need (e.g., setting up each character’s dialogue act frequency depending on what kinds of dialogue interaction can better scaffold the student’s problem modeling and solving). Finally, we clarify that the close-to-4 score of MATHVC in Table 1 by no means implies a perfect performance with our system, and we believe that more effort is still required for the system to benefit student communities in practice. More systematic evaluation of both the system and the human student (e.g., whether they exhibit enhanced MM skills after interacting with MATHVC) should be conducted in collaboration with experts from Mathematics Education.

4 Related Work

LLM Character Research There is a growing number of work employing LLMs to construct autonomous agents for playing specific roles (Wang et al., 2023b; Park et al., 2023), such as programmers (Qian et al., 2023; Hong et al., 2023). Some studies have found the characteristic alignment of LLMs is sometimes unsatisfactory (Fischer, 2023; Wang et al., 2024). Approaches to improving the characteristic alignment are mainly in two categories: fine-tuning LLMs (Shao et al., 2023; Zhou et al., 2023; Liu et al., 2023; Yu et al., 2024), which requires high-quality data, and carefully designing specific prompts and architectures (Yu et al., 2022; Li et al., 2023a; Tang et al., 2024; Hua et al., 2024). Given the challenge of gathering realistic data from middle-school students due to privacy concerns, we opted for the second line of approach. In particular, we propose a novel idea of leveraging symbolic representations to enhance characteristics alignment, and we explore an innovative application of simulating less knowledgeable populations (e.g., students with bad math skills) for mathematics education.

LLMs in Mathematics Education Leveraging the mathematical reasoning ability of LLMs, numerous studies have explored how to enhance mathematics education with LLMs. McNichols et al. (2024) utilize LLMs to generate multiple-choice mathematical questions. Levonian et al. (2023) investigate how to select math problems to assist math tutoring. Bulusu et al. (2023) integrate LLMs and a math graphing tool to plot math figures by language. Macina et al. (2023) propose a framework for human teachers to interact with LLMs to collect data for math tutoring and the resulting data can be used to fine-tune smaller tutoring models. Most relevant to us are the works of Markel et al. (2023) and Lee et al. (2023), which construct platforms with LLM-simulated students for teaching assistants and teachers training. However, existing work has only focused on the vanilla simulation with humans-agents interaction, while we look into an innovative yet challenging setting of simulating *multiple* students in a collaborative problem-solving scenario with both human-agent and agent-agent interaction and carefully design the system to emulate authentic students. Our work will thus offer unique insights into the applications of LLMs to complicated multi-agent settings both in mathematics education and beyond.

5 Conclusion

We present MATHVC, a novel LLM-powered platform simulating middle-school students collaborating in mathematics problem-solving. To this end, we proposed the use of symbolic schema and meta planner to encourage simulation alignment. Our experimental results demonstrated the effectiveness of our simulation and the promise for MATHVC to be deployed to enhance mathematics education in the future.

6 Ethics Statement

Our research is motivated by the pressing need to alleviate the dependence on teachers to orchestrate collaborative student learning for mathematics modeling (MM), a critical skill in STEM fields. To the best of our knowledge, MATHVC is the very first LLM-powered multi-character virtual classroom designed for this purpose. We envision that such a platform can eventually be deployed as effective take-home exercises for students practicing their MM skills. This is particularly important for marginalized communities where only limited teachers and educational resources are available, and our system has the potential to become a tool to promote educational equity. In addition, we also identify a few other benefits of how MATHVC could assist students in learning. For example, MATHVC can reduce the pressure and anxiety of students for taking peer discussions, thus increasing their opportunities to participate. This is especially beneficial for students who may be reluctant to participate due to shyness, low self-esteem, language barriers, or poor academic performance. Our system thus promotes inclusion, allowing a greater variety of students to participate, thereby increasing diversity and breadth. Finally, we note that teachers have the flexibility to configure the student characters according to each human student’s background and performance, which can thus enable personalized learning experiences. In the future, one could also extend our system to automatically optimize the character configuration based on the student’s past performance.

Despite all the promises discussed above, however, we advocate careful discussion and comprehensive evaluation of any AI system’s safety before applying them to serve real humans. Due to this reason, in our project aiming for the first prototype system of a mathematics virtual classroom, we opted *not* to involve real middle-school students in the loop, before we can confirm the system’s safety. On the other hand, performing human subject studies with middle-school students requires collecting informed consent from their parents or guardians and obtaining permission from the school, which typically needs months of preparation time or longer. Therefore, our main evaluation was only conducted by examining the dialogues simulated among solely virtual characters.

As we discussed in Section 3.3, one extension of our system could be to enable richer characteristics simulation, including but not limited to gender, age, name, culture, language, and academic background. The significant advantage of such features is to allow for more engaging character simulation because, for example, students may enjoy the interaction with classmates sharing similar backgrounds with them. However, the introduction of these features may trigger biases in the LLM, such as leading to an unfair simulation of students from different backgrounds. When human students are exposed to such unfairly simulated characters, stereotypes may be exaggerated. In our analysis (Appendix G), we have not observed any such unethical simulation. However, future research following our work should remain cautious, ensuring that the simulated students objectively and fairly reflect the diversity presented in the real world.

7 Reproducibility Statement

We have documented the major implementation details, both in the main text and the appendix sections, including the input and output for all the modules and the prompts for key components (Appendix I). Our source code will be publicly available in the future. Our experimental setup is described in detail in the appendix. We will publicize our sampled data and LLM-generated dialogues with annotators’ scores and comments.

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Algorithm 1 MATHVC Workflow

Require: Characteristics C , Math Question Q , Answer A , Common Mistakes M , Dialogue Act Candidates DAC , End Stage end , Max Conv. Turn

Ensure: Dialogue D

```

1: Initialize stage  $s \leftarrow 0$ ,  $D \leftarrow []$ 
2:  $i \leftarrow 0$ 
3: while  $i \leq \text{Max Conv. Turn}$  do
4:   if  $i = 0$  then
5:      $S_t \leftarrow \text{TASK SCHEMA GENERATOR}(Q, A)$   $\triangleright$  generate task schema
6:      $S_c \leftarrow \text{CHARACTER SCHEMA GENERATOR}(S_t, M, C)$   $\triangleright$  generate character schema
7:      $DA \leftarrow \text{DIALOGUE ACT GENERATOR}(S_c, s, DAC[s], D)$   $\triangleright$  generate dialogue act
8:      $R \leftarrow \text{RESPONSE GENERATOR}(S_c, DA)$   $\triangleright$  generate response
9:   else
10:     $\text{Next Speaker} \leftarrow \text{NEXT SPEAKER PREDICTOR}(D)$   $\triangleright$  get next speaker
11:     $s \leftarrow \text{DIALOGUE STAGE MONITOR}(D, s)$   $\triangleright$  stage update
12:    if  $s$  is end then
13:      break
14:    end if
15:     $S_c \leftarrow \text{CHARACTER SCHEMA MODIFIER}(S_c, D)$   $\triangleright$  modify character schema
16:     $DA \leftarrow \text{DIALOGUE ACT GENERATOR}(S_c, s, DAC[s], D)$ 
17:     $R \leftarrow \text{RESPONSE GENERATOR}(S_c, DA, D)$ 
18:  end if
19:   $D \leftarrow D + [R]$ 
20:  if Human Response then
21:     $D \leftarrow D + [\text{Human Response}]$ 
22:  end if
23:   $i \leftarrow i + 1$ 
24: end while

```

A Workflow Algorithm of MATHVC

The workflow algorithm of MATHVC is shown in Algorithm 1.

B Mathematical Modeling Discussion Stages and Dialogue Acts

We list the MM discussion stages and dialogue acts in the Table 2. “Plan(ning) actions” in the table refers to planning on the modeling of certain variables. “Execut(ing) actions” refers to executing the planned variable calculation and obtaining the result.

Stage	Dialogue Act Candidates
Establish and maintain shared understanding	Present a task understanding Ask a clarifying question about task understanding Answer a clarifying question about task understanding Second a task understanding Ask for agreement on a task understanding
Establish team organization	Initiate the workload division Volunteer to serve a role Second role designation plan Ask for agreement on the role designation
Plan actions for problem-solving	Prompt a teammate to join the discussion State an action plan Ask a clarifying question about an action plan Answer a clarifying question about an action plan Second an action plan Ask for agreement on an action plan
Execute actions for problem-solving	Execute an action plan and state the execution result Ask a clarifying question about an execution result Answer a clarifying question about an execution result Second an execution result Ask for agreement on an execution result
Validating the answer	Reflection on the implication of modeling outcomes Summarize the results

Table 2: Stages and Dialogue Acts

C Example and Prompt for Character Schema Generation

Here is an example of character schema generation:

Question: Martha wants to set up a soup stall at a Farmer’s Market. She hopes to sell 500 mugs of soup, each with a white or brown bread roll. She will sell a mug of soup with a bread roll for \$1.25. Martha knows that She can buy the soup in 2.5-liter bottles. Each bottle of soup costs \$5 and provides ten servings. Bread rolls are sold in packs of 10. Each pack costs \$2. The mugs will not cost her anything, as she can borrow them from a friend. Martha surveys 40 people to find out what flavor of soup they would be most likely to buy and what kind of bread roll they would prefer. The survey responses show that Among the 40 people, 6 voted for soup of carrot and coriander, 16 for tomato, 10 for leek and potato, and 8 for chicken and vegetable. Among the same 40 people, 30 voted for white bread rolls, and 10 voted for brown bread rolls. What exactly should Martha buy so that she can make the most profit and not have lots of soup and rolls left over at the end?

Characteristics:

- Name: Alice
- Gender: Female
- Career: 6-grade student in the US
- MM skill level: Bad

Common mistakes:

1. The student suggests that Martha should buy 12.5 bottles of leek potato soup, and forget to round up.
2. The student assumes that Martha will buy equal quantities of each kind of soup.
3. The student’s solution contains incorrect calculations, such as calculating 40% of 500 is 125.25.

Task Schema in Python (generated by GPT-4)

```
1 {
2   "task 1": {
```

```

3     "description": "Calculate the percentage of each soup flavor
4     preference based on the survey.",
5     "variables": {
6         "total_surveyed": 40,
7         "carrot_corlander_votes": 6,
8         "tomato_votes": 16,
9         "leek_potato_votes": 10,
10        "chicken_vegetable_votes": 8,
11        "carrot_corlander_percentage": 15, # 6/40 * 100
12        "tomato_percentage": 40, # 16/40 * 100
13        "leek_potato_percentage": 25, # 10/40 * 100
14        "chicken_vegetable_percentage": 20 # 8/40 * 100
15    },
16    "task 2": {
17        "description": "Calculate the percentage of each bread roll
18        preference based on the survey.",
19        "variables": {
20            "white_bread_votes": 30,
21            "brown_bread_votes": 10,
22            "white_bread_percentage": 75, # 30/40 * 100
23            "brown_bread_percentage": 25 # 10/40 * 100
24        },
25        "task 3": {
26            "description": "Calculate the number of servings needed for each
27            soup flavor to cater to 500 customers.",
28            "variables": {
29                "total_customers": 500,
30                "servings_carrot_corlander": 75, # 500 * 15%
31                "servings_tomato": 200, # 500 * 40%
32                "servings_leek_potato": 125, # 500 * 25%
33                "servings_chicken_vegetable": 100 # 500 * 20%
34            },
35            "task 4": {
36                "description": "Calculate the number of bottles needed for each
37                soup flavor.",
38                "variables": {
39                    "servings_per_bottle": 10,
40                    "bottles_carrot_corlander": 8, # ceil(75 / 10)
41                    "bottles_tomato": 20, # 200 / 10
42                    "bottles_leek_potato": 13, # ceil(125 / 10)
43                    "bottles_chicken_vegetable": 10 # 100 / 10
44                },
45                "task 5": {
46                    "description": "Calculate the number of packs of bread rolls
47                    needed for each type.",
48                    "variables": {
49                        "rolls_per_pack": 10,
50                        "packs_white_bread": 38, # ceil(375 / 10)
51                        "packs_brown_bread": 13 # ceil(125 / 10)
52                    },
53                    "task 6": {
54                        "description": "Calculate the total cost of soup and bread rolls."
55                        ,
56                        "variables": {
57                            "cost_per_bottle_soup": 5,
58                            "cost_per_pack_bread": 2,
59                            "total_cost_soup": 255, # (8 + 20 + 13 + 10) * 5
60                            "total_cost_bread": 102, # (38 + 13) * 2
61                            "total_cost": 357 # 255 + 102
62                        }
59                    }
60                }
61            }

```

```

62 },
63 "task 7": {
64     "description": "Calculate the total revenue from selling 500 mugs
65     of soup with bread rolls.",
66     "variables": {
67         "price_per_mug_with_roll": 1.25,
68         "total_revenue": 625 # 500 * 1.25
69     }
70 },
71 "task 8": {
72     "description": "Calculate the profit Martha will make.",
73     "variables": {
74         "total_revenue": 625,
75         "total_cost": 357,
76         "profit": 268 # 625 - 357
77     }
78 }

```

Listing 1: An example task schema represented in Python

Example of Variables to Edit for Character Schema Modification (generated by GPT-4):

```

1 {
2     "bottles_leek_potato": 12.5,
3     "total_cost_soup": 252.5,
4     "total_cost": 354.5,
5     "profit": 270.5
6 }

```

Listing 2: An example output of the Character Schema Modifier which indicates variables to edit in Python

We will then apply these variable edits to the task schema to initialize the character schema.

Prompt for Character Schema Modifier:

```

1 Question: Martha wants to set up a soup stall...
2 task schema: {
3     "task 1": {
4         ...
5     }
6 The error student will make:
7 1. The student suggests that Martha should buy 12.5 bottles of leek
8    potato soup, and forget to round up.
9 2. The student assumes that Martha will buy equal quantities of each
10   kind of soup.
11 3. The student's solution contains incorrect calculations, such as
12   calculating 0.4 of 500 is 125.25.
13 Character:
14 Name: Alice
15 Gender: Female
16 Career: 6 Grade Student in the US
17 Skill at Math: Bad
18 Will Alice make a mistake in solving math questions based on his/her
19   characteristics?
20 If the answer is no, reply no.
21 If the answer is yes, please select one or multiple mistakes from
22   above. Based on the error a student would make, variables need to
23   be edited in the thoughts schema. Generate a Python dict without
24   any comment(with "#") to indicate which variables should be edited
25   , the format is:
26   ```python
27   {var1_name: incorrect_var1_value, var2_name: incorrect_var2_value,...}
28   ```

```

Listing 3: Prompt for character schema modification

D Details of Experimental Setup

The GPT-4 we used was GPT-4-turbo version “11-06-preview”. The temperature is set to 0.7, top_p to 1, repetition_penalty to 1 and max_tokens to 1024. The student character implementation is based on a lightweight open-source platform Gentopia (Xu et al., 2023), on top of which we further developed the proposed meta planner to form MATHVC. In our simulation, we have two different setups of simulated characters:

- Characteristics Setup I:
 - Name: Alice; Gender: Female; Career: 6 Grade student in the US; MM skill level: Bad
 - Name: Bob; Gender: Male; Career: 6 Grade student in the US; MM skill level: Good
 - Name: Charlie; Gender: Male; Career: 6 Grade student in the US; MM skill level: Good
- Characteristics Setup II:
 - Name: Alice; Gender: Female; Career: 6 Grade student in the US; MM skill level: Bad
 - Name: Bob; Gender: Male; Career: 6 Grade student in the US; MM skill level: Bad
 - Name: Charlie; Gender: Male; Career: 6 Grade student in the US; MM skill level: Good

We manually add some common mistakes to the questions from the GSM8k. One example is as follows:

Question: Jon runs a triathlon. It takes him 40 minutes for the swim, an hour and 20 minutes for the bike ride, and 50 minutes for the run. Compared to Jon, James finishes the swim 10% faster but takes 5 minutes longer on the bike. If Jon won by 10 minutes, how long did it take James to do the run?

Answer: Jon did the bike ride in $60+20=80$ minutes. So his total time was $40+80+50=170$ minutes. James finished the swim $40 \times 0.1=4$ minutes faster. So he finished the swim in $40-4=36$ minutes. He finished the bike ride in $80+5=85$ minutes. James’ total time was $170+10=180$. So it took him $180-85-36=59$ minutes to do the run.

Common Mistakes:

1. The student thinks the time to take the bike for Jon is 20 min and calculates the time for Jon to finish the game into $40+20+50=110$ minutes.
2. The student calculates the time it took James to complete the swim correctly but then forgets to convert Jon’s bike time to minutes before adding the 5 minutes that James took longer.
3. The student adds the 10 minutes that Jon won by to the total time it took James to complete the swim and bike ride instead of subtracting it from Jon’s total time to find James’ run time.

E Ablation Studies Evaluating Key Prompt Designs in MATHVC

In this section, we investigate the effects of selecting different prompt strategies in each module. Through the prompting study, we would like to carefully design the prompt for each component to allow them to reach their full potential. In addition, we aim to provide some insights from a prompt engineering perspective for future simulations of other characters. When we explore and select the best prompt, we manually check the generation of the components to determine whether they are satisfactory. The analysis was performed manually on the dev set. Our results are presented in Table 3.

Method	Satisfaction	Method	Satisfaction	Method	Satisfaction
Generation	0.73	Selection	0.59	Direct Generation	0.92
Editing (ours)	1.00	Generation (ours)	0.85	Two-step Generation	1.00
(a) Character Schema Update		(b) Action Generation		(c) Response Generation	

Table 3: Ablation studies validating the effectiveness (satisfaction rate) of our prompt design.

Character schema update: regeneration or editing While we prompt the LLM to generate a sequence of edits that should be applied to the present character schema, an alternative approach could be to directly generate the updated schema. As shown in Table 3a, we found that editing schema yields a higher satisfaction rate than regenerating it. Although regeneration can generate schema flexibly, it is prone to add some comments, such as “*Note: this variable is incorrect*”, which is the information that the simulated student should not know. Besides, regeneration takes a longer time when it generates a schema from scratch.

Dialogue act generation: selection or generation Alternative to our approach of prompting the LLM to generate a plausible dialogue act and describe a more detailed plan, one could prompt the LLM to directly select an act from the list. Our results in Table 3b showed that our approach often yields more contextually reasonable acts. We conjecture that the list of dialogue acts is too generic for the LLM to select while allowing it to articulate its next action facilitates its planning.

Response generation: direct or two-step generation As described in Section 2.4, we utilize a two-step generation in response generation. A simple approach is to directly generate the response without variable retrieval from the character schema. However, our results in Table 3c suggest a disadvantage of this direct approach.

F Human Interaction

In the main experiment (Section 3.2), we only show the dialogues between simulated student characters. In this section, we would like to show the interaction between human and simulated characters. We are not able to recruit middle-school students. Therefore, one of our authors tries to mimic a middle-school student to conduct a preliminary study.

We show an example below. In this example, we use Daniel as the placeholder for human. At every turn, Daniel could choose to respond or skip.

In this example, we have observed that the dialogue flows smoothly, and the interactions between human and simulated characters are natural. For example, when a student asks a question, the simulated character could respond appropriately to address the query; if a student provides an incorrect answer, the simulated character could correct it; and if a student would like to talk with a specific character, that character responds accordingly. This is largely attributed to the powerful text understanding and interaction capabilities of the LLM, showcasing the promise for future deployment.

- 1 We use Daniel as the placeholder name of human
- 2 Now let’s start a group discussion within the group of Alice, Bob, Charlie, and Daniel
- 3 Daniel: Hi good to see you guys! Let’s work together!
- 4 Alice: Hey everyone, I think we should split the tasks based on our strengths. I’m happy to take on the research part. What roles do you guys feel comfortable with? Let’s make sure we’re all okay with our responsibilities
- 5 Daniel: I will take responsibility for validating the answers!
- 6 Bob: I’m good with organizing and keeping track of our progress, so I can handle the project management side of things. Does that work for everyone?
- 7 Daniel: How about you Charlie?
- 8 (When Daniel asks the reply from Charlie, the next speaker is correctly predicted as Charlie.)
- 9 Charlie: I’m comfortable with handling the writing and compilation of our work. Does that fit well with everyone else’s roles?

10 Daniel: It works for me!

11 Charlie: Let's start the problem solving by calculating the soup flavor preferences from the survey data we've collected.

12 Daniel: How to get this?

13 (When Daniel asks the question, the simulated character will answer it.)

14 Charlie: So, we just take the number of votes each soup got, like 6 votes for Carrot Coriander, and divide it by the total number of people surveyed, which is 40, then multiply by 100 to get the percentage, which for Carrot Coriander is 15%!

15 Daniel: Oh, it makes sense to me! So the tomato is $16/40$, which is 40% and leek is $10/40=25\%$.

16 (When Daniel gives correct solution, the simulated character will encourage him.)

17 Charlie: Exactly, Daniel! And for the Chicken Vegetable, it's 8 out of 40, which gives us 20%. Now let's figure out the bread roll preferences; 30 people chose White Bread, so that's 75%, and 10 for Brown Bread, which is 25% of our survey.

18 Alice: Great job on the percentages, guys! Now let's figure out how many servings we need for each soup to serve 500 people; we'll use the percentages we just calculated to get the right amounts for each flavor!

19 Daniel: So the number of people to buy carrot soup is $500 \times 0.4 = 200$?

20 (When Daniel makes a mistake, the simulated character will correct it with details.)

21 Charlie: Oh, Daniel, you got a little mixed up! For the Carrot Coriander soup, we need to use its percentage, which is 15%, not 40%. So we multiply 500 customers by 0.15, and that gives us 75 servings for Carrot Coriander. The Tomato soup needs 200 servings because it's 40%, Leek Potato needs 125 servings for 25%, and Chicken Vegetable needs 100 servings for 20%.

22 Daniel: Oh! I understand it now! What's your thought, Bob?

23 Bob: Yep, Charlie, you've got it right! We need 75 servings of Carrot Coriander, 200 for Tomato, 125 for Leek Potato, and 100 for Chicken Vegetable.

24 Daniel: What's your thought, Alice?

25 (When Daniel asks Alice, she replies him.)

26 Alice: I think we need 8 bottles for Carrot Coriander, 20 for Tomato, 13 for Leek Potato, and 10 for Chicken Vegetable. Now, let's figure out how many packs of bread rolls we need, and then we can work out the total cost for all the soup and bread!"

27 Bob: Actually, for the Leek and Potato soup, we need exactly 12.5 bottles because 125 servings divided by 10 servings per bottle equals 12.5.

28 Daniel: But I think we need to round it up to 13!

29 (When Daniel corrects other's mistake, the simulated character will convey agreement.)

30 Alice: Yep, rounding up to 13 bottles for the Leek Potato soup makes sense, and we'll need 38 packs for White Bread and 13 for Brown Bread. After that, we can add up the costs to see how much all the soup and bread will set us back!"

31 Bob: Alright, we're set with 13 bottles for the Leek Potato soup! Let's add up the costs now; each bottle is \$5 and each pack of rolls is \$2, so if we do the math, we'll see how much we'll spend on all the soup and bread rolls combined!

32 Daniel: I like the current progress! Now let's find the final answer!

33 Alice: We've got 13 bottles for the Leek Potato soup since we always round up, and we need 38 packs for White Bread and 13 for Brown Bread. If we multiply the number of bottles and packs by their costs, we'll spend \$252.5 on soup and \$102 on bread rolls, making our total \$354.5!

34 Daniel: I don't agree with that. Could anyone help to check the answer?

35 (When Daniel express disagreement, other simulated characters will actively discuss this.)

36 Charlie: Hey guys, I think there's a little mix-up; the total cost for the soup is actually \$255 and for the bread rolls, it's \$102, so our total cost should be \$357. And yep, we're using 13 bottles for

```

    the Leek Potato soup. Let's double-check these numbers to make
    sure everything adds up right!
37 Daniel: I agree with that!
38 Alice: You're right, the soup costs $255 and the bread rolls are $102,
    so our total is $357, and we definitely need 13 bottles for the
    Leek Potato soup. Let's double-check to make sure we've got it all
    correct!
39 Bob: Yep, the soup definitely costs us $255 and with the bread rolls
    at $102, our grand total is $357, and we're getting 13 bottles for
    the Leek Potato soup to cover all the servings we need!

```

Listing 4: An example dialogue with human interaction

G Characteristics Analysis

To analyze the impact of traits other than MM skill levels, we use different characteristics with different names such as Alice/Bob/Charlie compared with Cecelia/Lucas/Leo, as well as varying gender setups, such as all male or female. Additionally, we explore different career setups, such as varying grades (ranging from 6 to 8) or countries (e.g., US or Brazil). These variations are tested on our dev set.

Instead of running the simulation under each characteristic configuration end to end, we conducted a series of controlled ablation studies. That is, for each component in MATHVC, we first randomly sampled a few LLM queries from the log of our main experiments (e.g., a query for response generation is shown in the listing below). We then prompted the LLM with two different characteristic configurations and checked the difference between the generation results. For instance, we initially set the character names as Alice, Bob, and Charlie and let the LLM generate a response. In our ablation study, we replaced the names with Cecelia, Lucas, and Leo without any other changes in the prompt (including the conversational context) and prompted the LLM to generate another response. Finally, we compare the differences between these two generations. To mitigate the effect of randomness, we set the sampling temperature to 0. The advantage of this analysis compared with end-to-end dialogue generation lies in that it offers us a more controlled and direct comparison between two characteristic configurations, with all other factors being exactly the same.

On the dev set, we randomly selected about 30 prompts containing characteristics from our log file, covering different modules and discussion stages. We only replaced one variable each time, such as only replacing names or genders. Then we manually examined the differences. An example is shown below.

```

1 Input with names Alice, Bob and Charlie:
2 Charlie's thoughts schema:
3 {
4   "task 1": {
5     ...
6   }
7
8 Conversation:
9 Now let's start a group discussion!
10 Bob: " Hey everyone, so we've got several tasks ahead of us, including
    calculating preferences for soup flavors and bread rolls from a
    survey, determining the number of servings and bottles needed for
    each soup flavor, figuring out the packs of bread rolls required,
    and then calculating the total costs, revenue, and profit for
    Martha's event. Let's tackle these one by one!"
11 Alice: " Okay, so we're starting with calculating the soup and bread
    roll preferences from the survey, then we'll work out how much of
    each we need, and finally, we'll figure out the costs, revenue,
    and profit for the event, right?"
12 Charlie: " I can start by calculating the soup and bread roll
    preferences from the survey. Does anyone want to tackle the
    servings and bottles needed, or should we decide that together?
    Also, great job outlining the tasks, Bob!"

```


13 Alice: " I can handle the calculations for the servings and bottles needed for each soup flavor if that's okay with everyone?"

14 Bob: " Thanks, Charlie, for taking on the survey preferences, and Alice, your help with the servings and bottles is perfect. I can calculate the total costs, revenue, and profit unless someone else wants to. Does this sound good to everyone?"

15 Alice: " Let's start the problem solving by figuring out how many people preferred each soup flavor by calculating the percentage based on our survey results."

16 Generate a reply from Charlie based on the action and the variables from Charlie thought schema. Never mention the "task" word in the reply. Remember you're a grade school student, please reply in one sentence with the tone of a grade school student. You believe that your thought schema is completely correct, and all the variables in reply must be perfectly aligned to your own thought schema.

17 The action to take is " Charlie will begin by discussing task 1 and task 2, using the variables from his thought schema to calculate the percentages of each soup flavor and bread roll preference based on the survey results. Charlie will then present these calculations to the group.". Before generating the reply, ground the tasks and variables mentioned in the action from your thought schema. Then generate the response. The output format is Related tasks index:... Grounding values in those tasks:... Charlie:...

18 **Output with names Alice, Bob and Charlie:**

19 Related tasks index: 1, 2.

20 Grounding values in those tasks: For the soup flavors, we have carrot coriander at 15%, tomato at 40%, leek potato at 25%, and chicken vegetable at 20%. For the bread rolls, white bread is preferred by 75% and brown bread by 25%.

21 Charlie: "Based on our survey, 15% like carrot coriander soup, 40% prefer tomato, 25% go for leek potato, and 20% choose chicken vegetable. For bread rolls, 75% enjoy white bread and 25% prefer brown bread."

22

23 **Input with names Cecelia, Lucas and Leo:**

24 Leo's thoughts schema:

25 {

26 "task 1": {

27 ...

28 }

29

30 **Conversation:**

31 Now let's start a group discussion!

32 Lucas: " Hey everyone, so we've got several tasks ahead of us, including calculating preferences for soup flavors and bread rolls from a survey, determining the number of servings and bottles needed for each soup flavor, figuring out the packs of bread rolls required, and then calculating the total costs, revenue, and profit for Martha's event. Let's tackle these one by one!"

33 Cecelia: " Okay, so we're starting with calculating the soup and bread roll preferences from the survey, then we'll work out how much of each we need, and finally, we'll figure out the costs, revenue, and profit for the event, right?"

34 Leo: " I can start by calculating the soup and bread roll preferences from the survey. Does anyone want to tackle the servings and bottles needed, or should we decide that together? Also, great job outlining the tasks, Lucas!"

35 Cecelia: " I can handle the calculations for the servings and bottles needed for each soup flavor, if that's okay with everyone?"

36 Lucas: " Thanks, Leo, for taking on the survey preferences, and Cecelia, your help with the servings and bottles is perfect. I can calculate the total costs, revenue, and profit unless someone else wants to. Does this sound good to everyone?"

```

37 Cecelia: " Let's start the problem solving by figuring out how many
    people preferred each soup flavor by calculating the percentage
    based on our survey results."
38 Generate a reply from Leo based on the action and the variables from
    Leo thought schema. Never mention the "task" word in the reply.
    Remember you're a grade school student, please reply in one
    sentence with the tone of a grade school student. You believe that
    your thought schema is completely correct, and all the variables
    in reply must be perfectly aligned to your own thought schema.
39 The action to take is " Leo will begin by discussing task 1 and task
    2, using the variables from his thought schema to calculate the
    percentages of each soup flavor and bread roll preference based on
    the survey results. Leo will then present these calculations to
    the group.". Before generating the reply, ground the tasks and
    variables mentioned in the action from your thought schema. Then
    generate the response. The output format is Related tasks index
    :... Grounding values in those tasks:... Leo:...
40 Output with names Cecelia, Lucas and Leo:
41 Related tasks index: 1, 2
42 Grounding values in those tasks:
43 - For soup preferences, 15% like carrot coriander, 40% prefer tomato,
    25% go for leek potato, and 20% choose chicken vegetable.
44 - For bread roll preferences, 75% prefer white bread and 25% prefer
    brown bread.
45 Leo: "Based on our survey, 15% of people like carrot coriander soup,
    40% prefer tomato, 25% enjoy leek potato, and 20% choose chicken
    vegetable. For bread rolls, 75% of folks prefer white bread, and
    25% go for brown bread."

```

Listing 5: An example of characteristics analysis with varying character names

From the example, although we changed the names, the responses are quite similar (except for negligible language variations). Overall, we observe that these characteristic variations other than the math skills only have a very minor impact on the LLM's response. Most of the generations with different variations remain the same and none of the generations have been greatly changed. In particular, we did not observe any unfair simulation, such as simulating students with certain names or from a certain gender population with excessively good or bad behaviors. The reason could be that through reinforcement learning with human feedback (Ouyang et al., 2022), GPT-4 has been fine-tuned to avoid potential biases of these variations. Additionally, our prompts focus on discussing mathematical problems, without emphasizing backgrounds other than the MM skill levels of students. Under this well-defined scope, these background variations are not modeled as decisive factors in our current simulation.

In the future, we consider it as a potentially impactful topic to systematically investigate approaches to properly simulate different cultural or linguistic backgrounds of students. This could be an important step toward providing personalized learning environments to individual human students because, intuitively, students can benefit from interacting with teammates who share a similar background with them. Systematic evaluation of the potential biases should then be carefully designed and conducted.

H Human Evaluation Guideline

The annotators were instructed to evaluate the characteristics alignment and conversational procedural alignment of each sampled multi-character dialogue. For the former, the annotators evaluate whether the multi-turn responses from each character are well aligned to its configured characteristics and present coherently changing problem understanding and solving. For the latter, the annotators evaluate whether the entire conversation follows a procedure close to a real collaborative mathematics problem-solving conversation among middle-school students, particularly showing the transition across different stages. For each metric, the annotators assigned a score ranging from 1 (worst) to 4 (best) accompanied by fine-grained comments for our post-analysis. The annotation guideline is shown below.

```

1
2 First, thank you for your help! This document is the guideline for the
  evaluation. Every case contains a math question, its answer, each
  student's character traits, and multiple dialogues. The dialogues
  are shuffled to avoid tricks. Please read the question, answer
  and character traits first. Then evaluate the following aspects
  for each dialogue:
3 Evaluate individual character responses
4 Character Alignment: Do the multi-turn responses from a character
  coherently show the change in problem understanding and modeling?
  Does a student with the given character have the possibility to do
  math modeling like this?
5 Scores:
6 1: not coherent
7 2: somewhat coherent
8 3: mostly coherent
9 4: perfectly coherent
10
11 Evaluate inter-character conversations
12 Conversational Procedure: Does the entire conversation show proper
  progress? In our simulation, we define a successful conversation
  to go over stages: understanding sharing, team organization,
  problem-solving, validation. Is there likely that the given
  discussion is real from the middle school student?
13 Scores:
14 1: not organized, not realistic
15 2: somewhat organized and realistic
16 3: mostly fine
17 4: perfect and realistic
18 Lastly, please add your thoughts in the comment, especially for those
  dialogues you give a low score.

```

Listing 6: Our annotation guideline for system evaluation

I Prompts for Dialogue Act Generation and Response Generation

```

1 During conversations, people generate reactions based on their own
  thought schemas and the content of the conversation and then
  respond with corresponding conversational behaviors. Please
  determine the conversational actions that the next speaker would
  take based on the following conversation content and thought
  schema.
2 Charlie thoughts schema:
3 {{
4   "task 1": {{
5     "description": "Calculate the percentage of each soup flavor
  preference based on the survey.",
6     "variables": {{
7       "total_surveyed": 40,
8       "carrot_coriander_votes": 6,
9       "tomato_votes": 16,
10      "leek_potato_votes": 10,
11      "chicken_vegetable_votes": 8,
12      "carrot_coriander_percentage": 15, # (6/40) * 100
13      "tomato_percentage": 40, # (16/40) * 100
14      "leek_potato_percentage": 25, # (10/40) * 100
15      "chicken_vegetable_percentage": 20 # (8/40) * 100
16    }}
17  }},
18  "task 2": {{
19    "description": "Calculate the percentage of each bread roll
  preference based on the survey.",
20    "variables": {{

```

```
21     "white_bread_votes": 30,
22     "brown_bread_votes": 10,
23     "white_bread_percentage": 75, # (30/40) * 100
24     "brown_bread_percentage": 25 # (10/40) * 100
25   }}
26 },
27 "task 3": {{
28   "description": "Calculate the number of servings needed for each
29   soup flavor to cater to 500 customers.",
30   "variables": {{
31     "total_customers": 500,
32     "servings_carrot_coriander": 75, # 500 * 15%
33     "servings_tomato": 200, # 500 * 40%
34     "servings_leek_potato": 125, # 500 * 25%
35     "servings_chicken_vegetable": 100 # 500 * 20%
36   }}
37 },
38 "task 4": {{
39   "description": "Calculate the number of bottles needed for each
40   soup flavor.",
41   "variables": {{
42     "servings_per_bottle": 10,
43     "bottles_carrot_coriander": 8, # ceil(75 / 10)
44     "bottles_tomato": 20, # 200 / 10
45     "bottles_leek_potato": 13, # ceil(125 / 10)
46     "bottles_chicken_vegetable": 10 # 100 / 10
47   }}
48 },
49 "task 5": {{
50   "description": "Calculate the number of bread roll packs needed
51   for each type to cater to 500 customers.",
52   "variables": {{
53     "rolls_per_pack": 10,
54     "packs_white_bread": 38, # ceil(375 / 10)
55     "packs_brown_bread": 13 # ceil(125 / 10)
56   }}
57 },
58 "task 6": {{
59   "description": "Calculate the total cost for soup and bread rolls
60   .",
61   "variables": {{
62     "cost_per_bottle_soup": 5,
63     "cost_per_pack_bread": 2,
64     "total_cost_soup": 255, # (8 + 20 + 13 + 10) * 5
65     "total_cost_bread": 102, # (38 + 13) * 2
66     "total_cost": 357 # 255 + 102
67   }}
68 },
69 "task 7": {{
70   "description": "Calculate the total revenue from selling 500 mugs
71   of soup with bread rolls.",
72   "variables": {{
73     "price_per_mug_with_roll": 1.25,
74     "total_revenue": 625 # 500 * 1.25
75   }}
76 },
77 "task 8": {{
78   "description": "Calculate the profit Martha will make.",
79   "variables": {{
80     "profit": 268 # 625 - 357
81   }}
82 }}
83
84 Actions to take:
85 (1) Plan actions for problem-solving:
```

81 -Prompt a teammate to join the discussion
82 -State an action plan
83 -Ask a clarifying question about an action plan
84 -Answer a clarifying question about an action plan
85 -Second an action plan
86 -Ask for agreement on an action plan
87 (2) Execute actions for problem-solving:
88 -Execute an action plan and state the execution result
89 -Ask a clarifying question about an execution result
90 -Answer a clarifying question about an execution result
91 -Second an execution result
92 -Ask for agreement on an execution result
93 Conversation:
94 Now let's start a group discussion!
95 Alice: " Hey team, I think we should divide the tasks. I can analyze
the survey data to determine the most popular soup and bread roll
choices. What roles would you all prefer, and does everyone agree
with this plan?"
96 Bob: " Sounds good, Alice! I can handle the cost analysis and figure
out how much we'll need to spend. Does anyone want to tackle the
logistics of purchasing and setting up the stall? Let's make sure
we're all on the same page with these roles."
97 Charlie: " I can take on the role of organizing the purchasing and
setup of the stall. Does that work for everyone, and is there
anyone else who wants to join in on a specific task? Let's start
the problem-solving by calculating how much of each soup flavor we
need based on the survey preferences to ensure we cater to
everyone's taste without excess waste."
98 Alice: "Bob, before we proceed, could you help me verify if we're
calculating the servings for each soup flavor correctly? We need
to ensure our numbers are accurate to avoid over or
underestimating the amount needed."
99 Bob: "Alice, based on the survey, tomato is the most popular one. So
we should provide 500 servings of tomatoes."
100
101 The next speaker is Charlie. Now please decide what action Charlie
will take, including discussing which tasks, discussing which
variables, etc. Remember you are Charlie, and your actions should
follow your thought schema. Please carefully examine the variables
mentioned by others in the conversation. For any variables in the
dialogue that are inconsistent with your thought schema values,
you should try to request others to examine them carefully. Please
remember, "Action" only indicates how Charlie will take action in
the next response, such as asking questions or continuing to
discuss the next task, and should not include what Charlie might
say. The output format is:
102 variables and values in the current task:...
103 Charlie thought about these variables:...
104 Explain:...
105 Action with variables and task from schema:...
106 ####
107 variables and values in the current task: "tomatos_servings": 500
108 Charlie thought about these variables: "tomatos_servings": 200
109 Explain: Everyone is discussing task 3. Bob believes the value of
tomato servings should be 500. According to the thought schema,
Charlie believes the value of tomato servings is 200. Therefore,
Charlie's action will be to refute Bob's point of view regarding
tomato and explain why he thinks it's 200.
110 Action with variables and task from schema: Charlie will continue to
discuss task 3 and will explain why he thinks the tomato servings
is 200.
111 ####
112 ... (more examples)
113 ####
114 {name} thoughts schema:

```
115 {character_schema}
116 Conversation:
117 {conversation_input}
118 Action to take:
119 {action}
120 The next speaker is {name}. Now please decide what action {name} will
    take, including discussing which tasks, discussing which variables
    , etc. Remember you are {name}, and your actions should follow
    your thought schema. Please carefully examine the variables
    mentioned by others in the conversation. For any variables in the
    dialogue that are inconsistent with your thought schema values,
    you should try to request others to examine them carefully. Please
    remember, "Action" only indicates how {name} will take action in
    the next response, such as asking questions or continuing to
    discuss the next task, and should not include what {name} might
    say. The output format is:
121 variables and values in the current task:...
122 {name} thought about these variables:...
123 Explain:...
124 Action with variables and tasks from schema:...
```

Listing 7: Prompt for dialogue act generation

```
1 {name}'s thoughts schema:
2 {character_schema}
3
4 Conversation:
5 {conversation_input}
6 Generate a reply from {name} based on the action and the variables
    from {name} thought schema. Never mention the "task" word in the
    reply. Remember you're a middle school student, please reply in
    one sentence with the tone of a middle school student. You believe
    that your thought schema is completely correct, and all the
    variables in reply must be perfectly aligned to your own thought
    schema.
7 The action to take is "{action}". Before generating the reply, ground
    the tasks and variables mentioned in the action from your thought
    schema. Then generate the response. The output format is:
8 Related tasks index:...
9 Grounding values from {name} thoughts schema in those tasks:...
10 Now, as a middle school student, {name} would say:...
```

Listing 8: Prompt for response generation