# EXECUTABLE CODE ACTIONS ELICIT BETTER LLM AGENTS

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## Abstract

Large Language Model (LLM) agents, capable of performing a broad range of actions, such as invoking tools and controlling robots, show great potential in tackling real-world challenges. LLM agents are typically prompted to produce actions by generating JSON or text in a pre-defined format, which is usually limited by constrained action space (e.g., the scope of pre-defined tools) and restricted flexibility (e.g., inability to compose multiple tools). This work proposes to use executable Python code to consolidate LLM agents' actions into a unified action space (CodeAct). Integrated with a Python interpreter, CodeAct can execute code actions and dynamically revise prior actions or emit new actions upon new observations through multi-turn interactions. Our extensive analysis of 17 LLMs on API-Bank and a newly curated benchmark shows that CodeAct outperforms widely used alternatives (up to 20% higher success rate). The encouraging performance of CodeAct motivates us to build an open-source LLM agent that interacts with environments by executing interpretable code and collaborates with users using natural language. To this end, we collect an instruction-tuning dataset CodeActInstruct that consists of 7k multi-turn interactions using CodeAct. We show that it can be used with existing data to improve models in agent-oriented tasks without compromising their general capability. CodeActAgent, finetuned from Llama2 and Mistral, is integrated with Python interpreter and uniquely tailored to perform sophisticated tasks (e.g., model training) using existing libraries and autonomously self-debug.

## **1** INTRODUCTION

Large Language Models (LLMs) have emerged as a pivotal breakthrough in natural language processing (NLP). When augmented with *action* modules that allow access to APIs, their action space expands beyond conventional text processing, allowing LLMs to acquire capabilities such as tool invocation and memory management (Mialon et al., 2023; Schick et al., 2023) and venture into real-world tasks such as controlling robots (Ahn et al., 2022; Huang et al., 2023; Ma et al., 2023) and performing scientific experiments (Bran et al., 2023).

We inquire: *how to effectively expand LLM agents' action space for solving complex real-world problems?* Much existing research has examined using text (Yao et al., 2022b; Park et al., 2023, *inter alia*) or JSON (Qin et al., 2023b; Chase, 2022, *inter alia*) to produce actions (e.g., tool uses in Fig. 1 top left). However, both methods typically suffer from constrained scope of action spaces (actions are usually tailored for specific tasks) and restricted flexibility (e.g., inability to compose multiple tools in a single action). As an alternative approach, several work (Liang et al., 2022; Singh et al., 2023; Wang et al., 2023a) demonstrate the potential of using LLMs to generate code to control robots or game characters. However, they typically rely on pre-specified control primitives and hand-engineered prompts and, more importantly, struggle to dynamically adjust or emit actions based on new environmental observation and feedback.

This work proposes CodeAct, a general-purpose framework that allows LLMs to generate executable Python **code** as **act**ions (Fig. 1 top right). CodeAct is designed to handle a variety of applications and comes with unique advantages:

<sup>&</sup>lt;sup>1</sup>The code, data, model, and demo are available at https://github.com/xingyaoww/code-act.

## Preprint.

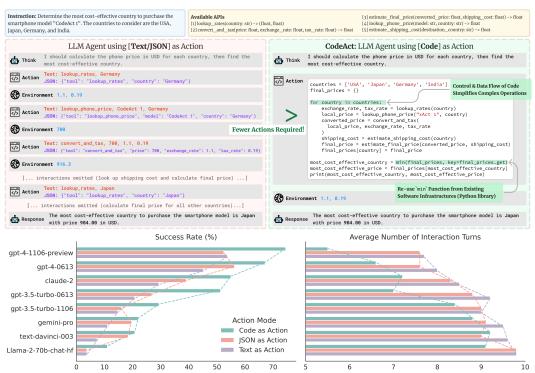


Figure 1: Comparison between CodeAct and Text / JSON as action. (top) Illustrative example comparing different actions. (bottom) Quantitative results on  $M^3$ ToolEval (§2.3).

- (1) Integrated with a Python interpreter, CodeAct can execute code actions and *dynamically adjust prior actions or emit new action* based on observations (e.g., code execution results) it receives through multiple turns of interactions.
- (2) Code actions allow LLM to leverage existing *software packages*. CodeAct can use readily available Python packages for an expanded action space instead of hand-crafted task-specific tools (Yuan et al., 2023; Shen et al., 2023). It also allows LLM to use automated feedback (e.g., error messages) implemented in most software to improve task-solving by self-debugging its generated code (Chen et al., 2023b; Wang et al., 2023d).
- (3) Code data is widely used in pre-training today's LLMs (Yang et al., 2024b). These models are already familiar with structured programming languages, allowing cost-effective adoption of CodeAct.
- (4) Compared to JSON and text with a pre-defined format, code inherently supports *control and data flow*, allowing for the storage of intermediate results as variables for reuse and the composition of multiple tools to perform complex logical operations (e.g., if-statements, for-loops) with *one* piece of code, thereby unlocking LLMs' potential to tackle complex tasks by leveraging its pre-trained knowledge of programming. In Fig. 1, an LLM using with CodeAct (top right) can apply the same sequence of tools (e.g., passing one tool's output as input to another tool using the data flow feature) to *all* inputs through for-loops (i.e., control flow feature) with *one* action; while text or JSON have to take action for every input (top left).

Our extensive experiments with 17 LLMs (including both open-source and proprietary ones) confirm the above benefits (3 & 4) of CodeAct. To demonstrate benefit (3), our first experiment (§2.2) compares CodeAct to baselines on basic tasks involving *atomic tool use* (i.e., only one tool is used per action), ablating the control and data flow advantage offered by CodeAct. The results show that, for most LLMs, CodeAct achieves comparable or better performance than the baselines. CodeAct's performance gains are more prominent on complex tasks, as demonstrated in our second experiment (benefit 4). We curate a new benchmark consisting of 82 human-curated tasks that typically require **m**ultiple calls to **m**ultiple tools in **m**ulti-turn interactions (M<sup>3</sup>ToolEval; §2.3). Problems in this benchmark often require intricate coordination and composition of multiple tools. With its strengths in control and data flow, CodeAct achieves up to a 20% absolute improvement over baselines on the success rate of solving the problems while requiring up to 30% fewer actions. These performance gains widen as the capabilities of the LLMs increase (Fig. 1 bottom).

The promising performance of CodeAct motivates an open-source LLM agent that can effectively act through CodeAct, and collaborate with humans through natural language. To this end, we collect

	CodeAct for LLM action	JSON or Text for LLM action
Availability of Data	✓ Large quantity of code available <sup>1</sup> for pre-training	XData curation required for particular format
Complex Operation (e.g., looping, composition of multiple tools)	✓ Natively supported via control and data flow	Requires careful engineering if feasible (e.g., define new tools to mimic if-statement)
Availability of Tools	$\checkmark$ Can directly use existing software packages <sup>2</sup>	Requires human effort to curate tools from scratch or existing software
Automated Feedback	✓ Feedback mechanism <sup>3</sup> (e.g., traceback) is already implemented as an infrastructure for most program- ming languages	Requires human effort to provide feedback or re- route feedback from the underlying programming language used to implement the tools

Table 1: The benefit of CodeAct compared to using Text/JSON for LLM action.

<sup>1</sup> Including code demonstrating useful behaviors for LLM agents (e.g., task decomposition, coordination of multiple function calls to different tools).

<sup>2</sup> Human-written Python packages covering a wide range of applications are available on https://pypi.org/.
 <sup>3</sup> For example, in Python, errors and exceptions (https://docs.python.org/3/tutorial/errors.html) are available. Most software provides error messages in natural language to help human programmers debug their code. CodeAct enables LLM to use them directly.

an instruction-tuning dataset CodeActInstruct consisting of 7k high-quality multi-turn interaction trajectories with CodeAct (§3.1). CodeActInstruct is motivated by a general agent framework consisting of agent, user, and environments (Fig. 2) and focuses on agent-environment interactions with the computer (information seeking, software package use, external memory) and the physical world (robot planning). On CodeActInstruct, we perform careful data selection to promote the capability of improving from multi-turn interaction (e.g., self-debug). We show that CodeActInstruct can be used with commonly used instruction tuning data to improve the models' performance in agent tasks without compromising their general capabilities (e.g., knowledge-based QA, coding, instruction following, §3.2). Our model, dubbed CodeActAgent, is finetuned from LLaMA-2 (Touvron et al., 2023) and Mistral-7B (Jiang et al., 2023) and improves on out-of-domain agent tasks with not only CodeAct, but also text action in a pre-defined format (§3.2).

CodeAct can further benefit from multi-turn interactions and existing software (benefit 1 & 2, §2.4). As shown in Fig. 3, CodeActAgent, designed for seamless integration with Python, can carry out sophisticated tasks (e.g., model training, data visualization) using existing Python packages. Error messages from the environment further enable it to rectify errors autonomously through self-debugging in multi-turn interaction. Thanks to LLM's extensive programming knowledge acquired during pre-training, these are achieved without needing in-context demonstrations, reducing the human efforts for adapting CodeActAgent to different tasks.

## 2 CODEACT MAKES LLMS BETTER AGENTS

In this section, we first describe CodeAct framework (§2.1) and provide empirical evidence that supports the choice of CodeAct. We focus on Python as the programming language for CodeAct due to its popularity (ranked top-1 at TIOBE Index (2024)) and numerous open-source packages. We aim to answer several research questions (RQs) using 17 off-the-shelf LLMs. In §2.2, we examine RQ1: Does LLMs' familiarity with code due to a large amount of code pre-training data bring CodeAct advantages over text and JSON? We discuss RQ2 in §2.3: Does CodeAct benefit from Python's innate control and data flow feature in complex problems? Finally, as an additional benefit, we discuss how using CodeAct further enhances LLM agents by enabling multi-turn interactions and allowing them to access existing software in §2.4 and Fig. 3.

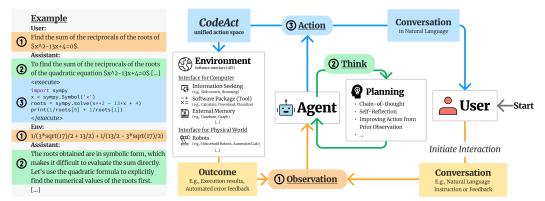


Figure 2: General agent multi-turn interaction framework that describes the role of CodeAct and motivates the construction of our data mixture. CodeActInstruct focuses on the *agent-environment* interactions and specifically filters for the self-improved *planning* behavior, while general conversation data we include focuses on *agent-user* interaction (§3.1).

## 2.1 WHAT IS CODEACT?

In Fig. 2, we first introduce a general multi-turn interaction framework for LLM agents' realworld usage that considers three roles (Yang et al., 2024c): agent, user, and environment. We define *interaction* as the information exchange between the agent and an external entity (user or environment). For each turn of interaction, the agent receives an observation (input) either from the user (e.g., natural language instruction) or the environment (e.g., code execution result), optionally planning for its action through chain-of-thought (Wei et al., 2022), and emits an action (output) to either user in natural language or the environment. CodeAct employs Python code to consolidate all actions for agent-environment interaction. In CodeAct, each emitted action to the environment is a piece of Python code, and the agent will receive outputs of code execution (e.g., results, errors) as *observation*. We include an example prompt of CodeAct in §E.

## 2.2 CODEACT SHOWS THE PROMISE AS A STRONG TOOL USE FRAMEWORK

In this section, we perform a controlled experiment to understand which format (text, JSON, CodeAct) is more likely to lead an LLM to generate correct *atomic* tool calls. The performance in this experiment reflects LLM's familiarity with the corresponding format. We hypothesize that using CodeAct to call tools is a more natural way to use tools for the models, which typically have extensive exposure to *code data* during their training.

Setup. We re-purpose API-Bank (Li et al., 2023) and test LLMs' API-calling performance, comparing CodeAct, JSON, and text actions. For each evaluation instance, we instruct LLM to generate one atomic tool call in the format of a Python function call, JSON object, or text expression in a predefined format. A concrete example is shown in Tab. A.6. We use API-Bank's level-1 instructions and the provided toolset. To evaluate API-calling, we follow their correctness metric, matching the ground-truth API outputs with the actual model-generated API's execution outputs.

Results. We present results in Tab. 2. For most LLMs, CodeAct achieves comparable or better performance even in atomic actions (the simplistic tool use scenario) where its control and data flow strengths are ablated. Compared to closed-source LLMs, CodeAct's improvements are more prominent in open-source models. Furthermore, code data is usually more accessible for finetuning open-source LLMs than the specialized JSON or text tool-calling format. Although JSON is consistently weaker than other approaches for open-source models, it achieves decent performance with closed-source LLMs, indicating that these closed-source models may have gone through targeted fine-tuning toward their JSON capabilities. These results suggest optimizing for CodeAct is a better route for open-source LLMs than alternatives to improve their tool-use capabilities, as they already show good initial CodeAct capability due to extensive exposure to code data during pre-training.

second-best is underlined.

Table 2: Atomic API call correctness on Table 3: Success rates (higher the better) and average turns API-Bank with different action format. required per instance (lower the better) on M<sup>3</sup>ToolEval. The best performance is **bolded**, and the The best results for each model are **bolded**, and the secondbest ones are underlined.

Correctness (%, ↑)				Success	Rate (%	<b>,</b> †)	Avg. Turns $(\downarrow)$			
Format of Action	CodeAct JSON Text		Text	Format of Action	CodeAct	JSON	Text	CodeAct	JSON	Text
Open-source 1	LMs				Open-sourc	e LLMs				
CodeLlama-7b-Instruct-hf	12.5	12.0	17.0	CodeLlama-7b-Instruct-hf	4.9	2.4	2.4	9.7	<u>9.9</u>	<u>9.9</u>
CodeLlama-13b-Instruct-hf	11.8	7.8	14.0	CodeLlama-13b-Instruct-hf	4.9	4.9	4.9	9.8	9.8	9.7
CodeLlama-34b-Instruct-hf	17.3	12.0	16.8	CodeLlama-34b-Instruct-hf	2.4	0.0	0.0	9.9	10.0	10.0
Llama-2-7b-chat-hf	28.8	11.3	25.8	Llama-2-7b-chat-hf	0.0	1.2	2.4	8.9	9.5	9.6
Llama-2-13b-chat-hf	38.1	8.5	37.3	Llama-2-13b-chat-hf	0.0	0.0	0.0	9.7	10.0	10.0
Llama-2-70b-chat-hf	<u>35.6</u>	14.3	37.6	Llama-2-70b-chat-hf	11.0	3.7	3.7	9.1	9.8	9.8
Mistral-7B-Instruct-v0.1	<u>2.5</u>	2.3	3.0	Mistral-7B-Instruct-v0.1	0.0	3.7	1.2	10.0	9.8	9.9
lemur-70b-chat-v1	58.6	46.6	56.1	lemur-70b-chat-v1	13.4	15.9	$1\overline{2.2}$	9.1	9.3	9.4
Closed-source	LLMs				Closed-sour	ce LLMs				
claude-2	76.7	59.4	73.7	claude-2	54.9	39.0	29.3	7.2	8.3	8.5
claude-instant-1	75.2	64.9	73.2	claude-instant-1	20.7	31.7	24.4	8.8	8.6	8.9
gemini-pro	70.4	73.2	71.2	gemini-pro	22.0	19.5	11.0	8.8	9.1	9.5
gpt-3.5-turbo-0613	74.4	73.9	73.4	gpt-3.5-turbo-0613	51.2	26.8	20.7	7.0	8.8	9.2
gpt-3.5-turbo-1106	75.4	78.4	73.4	gpt-3.5-turbo-1106	29.3	15.9	14.6	8.4	9.0	9.0
gpt-4-0613	75.4	82.0	74.4	gpt-4-0613	67.1	56.1	45.1	6.6	7.6	8.0
gpt-4-1106-preview	<u>76.7</u>	82.7	73.4	gpt-4-1106-preview	74.4	52.4	53.7	5.5	7.6	7.7
text-davinci-002	69.2	59.6	57.4	text-davinci-002	4.9	4.9	8.5	9.7	9.8	9.6
text-davinci-003	<u>75.4</u>	76.9	69.7	text-davinci-003	20.7	18.3	7.3	9.2	9.0	9.6
Frequency of Best-Perfo	rming Forma	nt ↑		Frequency	of Best-perfor	rming Fo	rmat †			
Open-source	4	0	4	Open-source	5	4	3	6	1	1
Closed-source	<u>4</u>	5	0	Closed-source	7	1	1	6	$\frac{1}{2}$	1
Overall	8	<u>5</u>	4	Overall	12	5	$\overline{4}$	12	3	2

## 2.3 CODEACT GETS MORE DONE WITH FEWER INTERACTIONS

In this section, we investigate whether LLM agents can benefit from the control and data flow of code on problems that require complex patterns of tool use.

 $M^{3}$ ToolEval. As shown in Tab. A.7, to the best of our knowledge, no existing tool-use benchmarks contain complex tasks requiring the composition of multiple tools while supporting evaluating different action formats. Hence, we curate a benchmark  $M^{3}$ ToolEval to fill this gap, which evaluates LLMs' capabilities in solving complex tasks that typically require **m**ultiple calls to **m**ultiple tools in **m**ulti-turn interactions. It contains 82 human-curated instances, spanning tasks including web browsing, finance, travel itinerary planning, science, and information processing. Each domain is accompanied by a unique set of manually crafted tools. We intentionally keep the prompt simple (examples in §F) and avoid providing any demonstration to test the LLM's zero-shot ability to use tools, similar to how a novice user without knowledge of few-shot prompting would use the model.

**Setup.** We allow the model to generate fully functional Python code that enables control and data flow (e.g., if-statement, for-loop). We follow the action format for JSON and text described in Tab. A.6. Within each turn, the model can either emit an *action* or propose an *answer* to be verified by an exact match with the ground-truth solution. The interaction will terminate when a maximum of 10 interaction turns are reached or a correct solution has been submitted, similar to Wang et al. (2023e).

**Metric.** We measure the *success rate* by calculating the percentage of the model proposed answers that match the ground-truth solutions. We also include the *avg. turns* metric: the average number of turns on all evaluated instances.

Quantitative Results on  $M^3$ ToolEval. We include full results in Tab. 3 and a subset of results for visualization in Fig. 1. CodeAct generally has a higher task success rate (12 out of 17 evaluated LLMs), similar to the trend in §2.2. Moreover, using CodeAct requires a lower average number of turns (12 out of 17 evaluated LLMs). For example, the best model gpt-4-1106-preview achieves a 20.7% absolute improvement compared to the next best action format (text) while requiring 2.1 fewer interaction turns on average. However, there is still a significant gap in terms of absolute CodeAct performance between open- and closed-source LLMs as the best open-source model achieving 13.4% while the best closed-source model gpt-4-1106-preview 74.4%. This is potentially due to open-source models' weak task-solving capability and inability to follow complex instructions without demonstration, suggesting an urgent need to improve open-source LLMs for practical, real-world tasks under the zero-shot setting.

## 2.4 CODEACT BENEFITS FROM MULTI-TURN INTERACTIONS AND EXISTING SOFTWARE PACKAGES

In Fig. 3, we show how an LLM agent can integrate with Python (i.e., CodeActAgent we trained in §3.2) and use existing software to perform complex tasks in multi-turn interactions. Thanks to its extensive knowledge of Python learned during pre-training, the LLM agent can automatically import the correct *Python libraries* to solve tasks without requiring user-provided tools or demonstrations. As illustrated in Fig. 3, CodeActAgent can use Pandas to download and process tabular data, use Scikit-Learn for machine learning train-test data split and regression model training, and use Matplotlib for data visualization. Furthermore, using the interactive Python interpreter for code execution allows automated error messages that help the LLM agent 'self-debug' their actions in a *multi-turn interaction* and eventually complete the human user's request correctly.

## 3 EMPOWERING OPEN-SOURCE LLM AGENT TO BE BETTER AT CODEACT

The promising results achieved by CodeAct motivate us to build an open-source LLM agent that can both interact with environments through CodeAct and communicate with humans using language. To improve open-source LLMs' CodeAct capability, in §3.1, we introduce CodeActInstruct, an instruction finetuning dataset that contains agent-environment interaction trajectories. We discuss data selection procedures in §3.1 to promote improvement from interaction behavior. Additionally, we show that CodeAct can be used together with existing agent-user conversation data (§3.1) to balance the dialog capability of the resulting LLM. Our model CodeActAgent, finetuned from LLaMA-2 (Touvron et al., 2023) and Mistral-7B (Jiang et al., 2023) on a mixture of CodeActInstruct and general

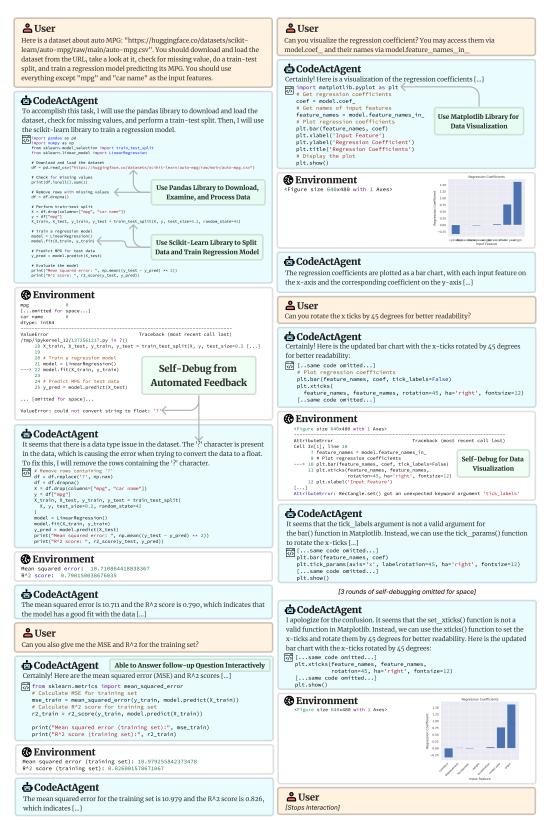


Figure 3: Example multi-turn interaction with Python packages using CodeActAgent (Mistral-7b). No in-context demonstrations are provided to the model. Some messages are omitted for space. See https://chat.xwang.dev/r/Vqn108G for complete interaction.

conversations, improves CodeAct performances without hurting LLM's general performance on a diverse suite of tasks ( $\S$ 3.2).

## 3.1 CODEACTINSTRUCT: AGENT-ENVIRONMENT INTERACTIONS

We consider four main use cases in agent-environment interaction and repurpose five existing datasets across different domains to generate trajectories:

- Information Seeking: We use a training subset of HotpotQA (Yang et al., 2018) to generate information-seeking trajectories, where LLMs use the wikipedia\_search API (provided as a Python function) to search for information to answer questions.
- **Software Package (Tool) Usage:** We use the training set of code generation problems in APPS (Hendrycks et al., 2021a) and math problems in MATH (Hendrycks et al., 2021b). The code generation tasks already involve importing packages and/or creating new tools by defining a new Python function. For MATH, we provide an in-context demonstration of importing Python packages (e.g., sympy for symbolic math) for problem-solving.
- External Memory: We repurpose the training subset of WikiTableQuestion (Pasupat & Liang, 2015) and tweak it into two variants of tabular reasoning tasks that require accessing external memory: (1) SQL-based, requiring the LLM to interact with an SQL database through sqlite3 package to answer the question via SQL execution; (2) Pandas-based, requiring the model to interact with pandas tables to perform data operations (e.g., select, filter). Examples of instructions can be found in §G.3.1.
- **Robot Planning:** We use ALFWorld (Shridhar et al., 2020), a text-only embodied environment simulator, to generate trajectories that use robot-control APIs (repurposed as Python function) to complete household tasks. Following MINT (Wang et al., 2023e), we provide an in-context demonstration to encourage the use of for-loop and if-statement code blocks to automate repetitive operations (e.g., searching for items by visiting different locations).

**Data Down-sampling.** We down-sample each dataset by keeping only the most challenging instances, aiming to make trajectory generation more efficient and cost-effective. Furthermore, it also helps remove simple instances that existing LLMs can already solve. The statistics of the filtered dataset can be found in Tab. A.9. Please refer to §G.1 for details about the down-sample process.

**Repurpose Data for Multi-turn Interaction.** Some datasets (APPS, MATH, WikiTableQuestions) are initially single-turn problems that expect *one* solution per instruction, whereas, in a realistic agent use case, we often require multi-turn interaction to complete each task (Fig. 1 top). Following MINT (Wang et al., 2023e), we repurpose single-turn problems into multi-turn ones by allowing LLM to interact with the environment for multiple turns before it decides to submit one solution for evaluation. Specifically for code generation problems, we provide an in-context example to guide LLMs to test their solution on provided test cases before they submit the solution. Metrics from the original data will evaluate the submitted solution to determine its correctness. We include examples in §G.3.

**Trajectory Generation.** We use MINT's evaluation framework (Wang et al., 2023e) to generate interaction trajectories for the aforementioned datasets and determine the correctness of each trajectory. We run gpt-3.5-turbo-0613 from OpenAI, claude-1-instant and claude-2 from Anthropic on down-sampled data, except code generation, which we use a longer-context version of GPT-3.5 (gpt-3.5-turbo-0613-16k) due to the long-context requirement of the self-debugging process. On a subset of problems that none of these models can solve, we use gpt-4-0613 to generate trajectories.

**Enhancing Agent's Capabilities of Improving from Interaction.** We select a high-quality subset of all the generated trajectories from CodeActInstruct to promote the agent's ability to improve the next action based on prior observations (e.g., self-debugging from code execution error message, a planning capability in Fig. 2). To achieve this, we selectively preserve those trajectories wherein the model initially encounters errors but rectifies these inaccuracies in later interactions. For these instances, the LLM typically engages in self-reflection following the initial error, thereby proactively enhancing its future actions. Other filtering details are discussed in §G.2. On all trajectories generated, we keep 411 trajectories from gpt-4-0613 and 6728 trajectories from gpt-3.5 and claude. The statistics of the resulting dataset CodeActInstruct are shown in Tab. 4.

**Comparing CodeActInstruct with Prior Work.** Compared with prior work AgentInstruct (Zeng et al., 2023) and FireAct (Chen et al., 2023a) that mainly focus using text as action, CodeActInstruct results in models that are more practical in real-world implementation, as such models using CodeAct can directly interact with Python interpreters and open-source toolkits (Fig. 3), reducing the development effort for action parsing and tool creations. CodeActInstruct is systematically constructed following the general agent framework (Fig. 2). It covers diverse domains (e.g., compared

Data Mixture	Data Type	Data Name	# of Data Instances	# of Total Tokens	Avg. Tokens Per Instance
Prior Work	-	FireAct (Chen et al., 2023a)	2,063	542, 176	262.81
THOI WOIK	-	AgentInstruct (Zeng et al., 2023)	1,866	2,517,785	1349.30
	Information Seeking	HotpotQA (Yang et al., 2018)	1,664	2,472,227	1485.71
	Software Packages (Tool)	MATH (Math, (Hendrycks et al., 2021b))	1,732	1,719,467	992.76
	Software Packages (Tool)	APPS (Code, (Hendrycks et al., 2021a))	647	1,235,472	1909.54
CodeActInstruct (Ours)	External Memory	WikiTableQuestion (Pasupat & Liang, 2015)	1,065	1, 316, 246	1235.91
	Robot Planning	ALFWorld (Shridhar et al., 2020)	2,031	3, 838, 269	1889.84
		Total	7,139	10, 581, 681	1482.24
	Single-Turn Reasoning	OpenOrca (Sub-sampled, (Lian et al., 2023))	50,000	14,034,152	280.68
	Multi-Turn Conversations	ShareGPT (Sub-sampled, (Anonymous, 2023))	10,000	17,933,861	1793.39
General Conversation	Multi-Turn Conversations	ShareGPT (GPT-4, (OpenChat, 2023))	4,583	18, 195, 878	3970.30
	Multi-turn Reasoning	CapyBara (LDJnr, 2023)	4,647	4,982,435	1072.18
		Total	69,230	55, 146, 326	796.57

Table 4: Statistics of our training mixture and comparison with prior work. Please refer to §3.1 for details about CodeActInstruct and general conversation data. Token statistics are computed using Llama-2 tokenizer.

Table 5: Evaluation results for CodeActAgent. The best results among all open-source LLMs are **bolded**, and the second-best results are <u>underlined</u>. ID and OD stand for in-domain and out-of-domain evaluation correspondingly. Overall averaged performance normalizes the MT-Bench score to be consistent with other tasks and excludes in-domain tasks for fair comparison.

						-				
			Agent Tasks				Generi	c Tasks		Overal
		Code as Ac	tion	Text as Act	tion (OD)		(0	D)		Average
Size	MINT (ID)	MINT (OD)	M <sup>3</sup> ToolEval (OD)	Miniwob++	SciWorld	MMLU	HumanEval	GSM8K	MTBench	_
			Open-source LL	Ms (LLaMA-2-b	ased)					
7B	-*	_*	-*	-*	_*	45.3	12.8	14.6	-*	_*
7B	3.2	11.0	0.0	0.0	5.9	48.0	13.9	27.7	6.3	21.1
7B	0.0	0.3	0.0	0.0	6.8	44.1	3.5	12.4	4.5	14.0
7B	8.7	6.1		28.9	13.7	48.7	15.4	24.6	6.1	24.8
7B	<u>51.3</u>	<u>20.4</u>	0.0	25.5	17.6	50.6	18.1	38.3	7.5	<u>30.</u>
			Open-source L	LMs (Mistral-ba	sed)					-
7B	-*	_*	-*	-*	-*	60.1	30.5	52.1	-*	_*
7B	18.8	9.7	0.0	0.5	4.0	53.8	29.3	43.3	6.4	25.6
7B	57.4	32.4	$1\overline{2.2}$	46.2	15.9	59.1	34.7	58.0	8.2	42.5
			Closed-	source LLMs						
-	33.9	38.2	51.2	66.7	21.2	70.0	48.1	57.1	7.9	54.0
-	68.6	70.2	67.1	69.4	36.4	86.4	67.0	87.1	9.0	71.7
	7B 7B 7B 7B 7B 7B 7B 7B	7B         -*           7B         3.2           7B         0.0           7B         51.3           7B         -           7B         18.8           7B         57.4           -         33.9	Size         MINT (ID)         MINT (OD)           7B         -*         -*           7B         3.2         11.0           7B         0.0         0.3           7B         8.7         6.1           7B         51.3         20.4           7B         -*         -*           7B         18.8         9.7           7B         57.4         32.4           -         33.9         38.2	Tode as Action           Size         Open-source LL           7B         -*         -*         -*           7B         3.2         11.0         0.0           7B         0.0         0.3         0.0           7B         51.3         20.4         0.0           7B         18.8         9.7         0.0           7B         57.4         32.4         12.2           7B         33.9         38.2         51.2	Text as Action           Text as Action           Gene as Action           MINT (ID)         MINT (OD)         M <sup>3</sup> ToolEval (OD)         Miniwob++           7B         .*         .*         Open-source LLMs (LLaMA-2-b)           7B           Open-source LLMs (LLaMA-2-b)           7B         0.0         0.3         0.0         0.0           7B         0.0         0.3         0.0         0.0           7B         51.3         20.4         0.0         28.9           7B         51.3         20.4         0.0         25.5           7B         18.8         9.7         0.0         0.5           7B         18.8         9.7         0.0         0.5           7B         57.4         32.4         12.2         46.2           Closed-source LLMs	Text as Action (OD)           Size         MINT (ID)         MINT (OD)         M <sup>3</sup> ToolEval (OD)         Miniwob++         SciWorld           7B         -*         *         -*         *         *         *         *         *         *         *         *         *         *         *         *         *         *         *         *         *         *	Agent Tasks           Code as Action         Text as Action (OD)           Size         MINT (ID)         MINT (OD)         Minivob++         SciWorld         MMLU           7B         -*         -*         -*         45.3         45.3           7B         3.2         11.0         0.0         0.0         5.9         48.0           7B         0.0         0.3         0.0         0.0         6.8         44.1           7B         51.3         20.4         0.0         25.5         17.6         50.6           7B         -*         -*         -*         -*         -*         60.1           7B         51.3         20.4         0.0         0.5         40.5         50.6           7B         51.3         20.4         0.0         0.5         40.5         50.6           7B         51.3         20.4         0.0         0.5         40.5         50.6           7B         51.3         20.4         12.2         46.2         15.9         59.1           7B         18.8         9.7         0.0         0.5         40.5         53.8         78         57.4         32.4         12.2 <td>Agent Tasks         Generic           Code as Action         Text as Action (OD)         (OO)           Size         MINT (ID)         MINT (OD)         M<sup>3</sup>ToolEval (OD)         Minivob++         SciWorld         MMLU         HumanEval           7B         -*         -*         -*         -*         45.3         12.8           7B         3.2         11.0         0.0         0.0         5.9         48.0         13.9           7B         0.0         0.3         0.0         0.0         6.8         44.1         3.5           7B         5.1.3         20.4         0.0         25.5         17.6         50.6         18.1           7B         -*         -*         -*         -*         -*         6.1         30.5           7B         51.3         20.4         0.0         25.5         17.6         50.6         18.1           7B         -*         -*         -*         -*         -*         6.1         30.5           7B         18.8         9.7         0.0         0.5         4.0         53.8         29.3           7B         57.4         32.4         12.2         46.2         <td< td=""><td><math display="block">\begin{tabular}{ c c c c c c c } \hline &amp; Agent Tasks &amp; Generic Tasks \\ \hline \hline Code as Action &amp; Text as Action (OD) &amp; (OD) \\ \hline \\ Size &amp; MINT (ID) &amp; MINT (OD) &amp; M^3 ToolEval (OD) &amp; Miniwob++ &amp; SciWorld &amp; MMLU &amp; HumanEval &amp; GSM8K \\ \hline \\ TB &amp; .* &amp; .* &amp; &amp; &amp; &amp; &amp; &amp; .</math></td><td><math display="block">\begin{tabular}{ c c c c c c c c c c c c c c c c c c c</math></td></td<></td>	Agent Tasks         Generic           Code as Action         Text as Action (OD)         (OO)           Size         MINT (ID)         MINT (OD)         M <sup>3</sup> ToolEval (OD)         Minivob++         SciWorld         MMLU         HumanEval           7B         -*         -*         -*         -*         45.3         12.8           7B         3.2         11.0         0.0         0.0         5.9         48.0         13.9           7B         0.0         0.3         0.0         0.0         6.8         44.1         3.5           7B         5.1.3         20.4         0.0         25.5         17.6         50.6         18.1           7B         -*         -*         -*         -*         -*         6.1         30.5           7B         51.3         20.4         0.0         25.5         17.6         50.6         18.1           7B         -*         -*         -*         -*         -*         6.1         30.5           7B         18.8         9.7         0.0         0.5         4.0         53.8         29.3           7B         57.4         32.4         12.2         46.2 <td< td=""><td><math display="block">\begin{tabular}{ c c c c c c c } \hline &amp; Agent Tasks &amp; Generic Tasks \\ \hline \hline Code as Action &amp; Text as Action (OD) &amp; (OD) \\ \hline \\ Size &amp; MINT (ID) &amp; MINT (OD) &amp; M^3 ToolEval (OD) &amp; Miniwob++ &amp; SciWorld &amp; MMLU &amp; HumanEval &amp; GSM8K \\ \hline \\ TB &amp; .* &amp; .* &amp; &amp; &amp; &amp; &amp; &amp; .</math></td><td><math display="block">\begin{tabular}{ c c c c c c c c c c c c c c c c c c c</math></td></td<>	$\begin{tabular}{ c c c c c c c } \hline & Agent Tasks & Generic Tasks \\ \hline \hline Code as Action & Text as Action (OD) & (OD) \\ \hline \\ Size & MINT (ID) & MINT (OD) & M^3 ToolEval (OD) & Miniwob++ & SciWorld & MMLU & HumanEval & GSM8K \\ \hline \\ TB & .* & .* & & & & & & .$	$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$

\* Some results are only available with instruction-tuned models.

to FireAct that only considers QA-task and search API), contains quality data (e.g., promotes agent's capability of self-debug) and of larger size (3.8x / 3.5x more data trajectories and 5x / 19x more tokens compared to AgentInstruct / FireAct respectively in Tab. 4). As we empirically show in Tab. 5, the resulting model (same backbone) of CodeActInstruct achieves 24% and 119% relative improvement compared to AgentInstruct and FireAct.

**CodeActInstruct Can Be Used With Existing Agent-User Conversation Data.** We use a subsampled set of OpenOrca (Lian et al., 2023) that focuses on single-turn chain-of-thought (CoT) reasoning, ShareGPT (Anonymous, 2023; OpenChat, 2023) from two sources that contain multi-turn conversations between human and LLM, and CapyBara (LDJnr, 2023) that focuses on reasoning in multi-turn conversations. Statistics and down-sampling details can be found in Tab. 4 and §C.

## 3.2 CODEACTAGENT

We fine-tune Llama-2 7B (Touvron et al., 2023) and Mistral 7B (Jiang et al., 2023) on a mixture of CodeActInstruct and general conversations (Tab. 4) to obtain CodeActAgent.

**Training Setup.** We perform full-parameter supervised fine-tuning with a sequence length of 4,096 tokens for Llama-2 and 16,384 for Mistral. Please refer to §D for more details.

**Evaluation Setup.** We use MINT (Wang et al., 2023e) to evaluate LLMs with CodeAct on a diverse range of agent tasks. CodeActAgent has some training domains overlapping with MINT's evaluation (i.e., MINT includes ALFWorld and MATH), hence we report separate numbers for MINT's inand out-of-domain performance. Unless otherwise specified, we measure MINT tasks' success rates with interaction turn k = 5. We also evaluate out-of-domain agent tasks using text actions from MiniWob++ (computer tasks, Kim et al. (2023)) and ScienceWorld (text-based simulator for elementary science curriculum, Wang et al. (2022a)) to test whether CodeActAgent can generalize to different action formats. Finally, we include a suite of general LLM evaluation tasks to assess general capability: MMLU (Hendrycks et al., 2020) for knowledge-based QA, HumanEval (Chen et al., 2021) for single-turn code-generation, GSM8K (Cobbe et al., 2021) for single-turn tool-free math reasoning, and MTBench (Zheng et al., 2023) for instruction-following. **CodeActAgent Excels in CodeAct Task.** As shown in Tab. 5, CodeActAgent (both variants) perform better than all evaluated open-source LLMs on both the in- and out-of-domain subsets of MINT. On M<sup>3</sup>ToolEval, we find CodeActAgent (Mistral) outperforms open-source LLMs of similar size (7B and 13B) and even reaches similar performance to those 70B models (Tab. 3). Surprisingly, no improvement is observed for the Llama-2 variant. We discuss potential reasons in §H.

**CodeActAgent Generalizes to Text Action.** When evaluated on out-of-domain text actions, Code-ActAgent (LLaMA2, 7B), which has never been optimized for text action, achieves comparable performance to AgentLM-7B (Zeng et al., 2023) which has explicit tuning for text actions.

**CodeActAgent Maintains or Improves the Performance on General LLM Tasks.** In Tab. 5, we find that CodeActAgent (both variants) performs better on generic LLM tasks we tested, except for a slight degradation on MMLU for CodeActAgent (Mistral, 7B).

**Ablation Study.** Tab. A.8 presents ablation experiments to determine the importance of CodeActInstruct and general conversations. Both CodeActInstruct and general conversations contribute to agent tasks, while general conversations are essential to maintain performance on general tasks.

## 4 RELATED WORK

## 4.1 ACTION MODULE IN LLM AGENTS

As detailed in Wang et al. (2023b), LLM-based autonomous agents are typically structured around four components: customized profiles (Park et al., 2023; Qian et al., 2023), long-term memory capabilities (Zhu et al., 2023; Fischer, 2023), reasoning and planning algorithms (Wei et al., 2022; Chen et al., 2023d), and, most crucially, action modules. The action modules are key to facilitating LLM agents to effectively interact with external entities, including humans (Lee et al., 2022) and tools (Qin et al., 2023a) in the environment (Wang et al., 2023e; Yang et al., 2024a). In this study, we address the critical problem of standardizing the action space for LLM agents. We further discuss the difference between CodeAct and the line of work that uses code generation for problem-solving in §A. We notice a concurrent study TaskWeaver (Qiao et al., 2023) similarly endorses the use of code. We discuss the principal distinctions in §B.

## 4.2 IMPROVING LLM AGENTS

Two primary methods for enhancing LLM agents are prompt engineering and instruction tuning, as surveyed by Wang et al. (2023b). For *prompt engineering* (Liu et al., 2023a), numerous strategies have been introduced to improve the chain-of-thought reasoning (Wei et al., 2022), including self-consistency-based reasoning (Wang et al., 2022b; Chen et al., 2023d) and tree-based approaches (Yao et al., 2023a). Moreover, LLMs can be strategically prompted to reflect on previous plans (Yao et al., 2023b; Wang et al., 2023f; Zhang et al., 2023), enabling them to refine initial actions through trial and error. Contrast to prompt engineering, *instruction tuning* intrinsically enhances LLMs (Chung et al., 2022), particularly in their agent capabilities (Zeng et al., 2023; Chen et al., 2023a). For effective training, human annotators can curate expert demonstrations for specific agent tasks, such as web browsing (Yao et al., 2022a; Nakano et al., 2021). To minimize human annotation efforts, prior work creates synthetic datasets using stronger LLMs to distill agent capabilities into local models, focusing on tool usage (Qin et al., 2023b), interaction (Chen et al., 2023c), and social skills (Liu et al., 2023b). CodeActInstruct aligns with the latter approach and creates datasets using stronger LLMs.

## 5 CONCLUSIONS

This work introduces CodeAct that employs executable Python code for the LLM agent's action, which is advantageous over using text or JSON action, especially in complex scenarios. We collect CodeAct-focused multi-turn interaction trajectories CodeActInstruct for instruction tuning, and train CodeActAgent that is specially designed for seamless integration with Python and can execute sophisticated tasks (e.g., model training) leveraging existing Python packages and autonomously rectifying errors through self-debugging.

## BROADER IMPACTS, LIMITATIONS, AND FUTURE WORK

This paper presents work whose goal is to advance LLM-based autonomous agents that can communicate with humans through natural language and assist human users by performing tasks in environments on behalf of humans. In this section, we discuss potential societal consequences, limitations, and future work related to our work and its goal.

CodeActAgent is an initial prototype of an autonomous agent and still has several practical limitations. For example, it may suffer from hallucination commonly seen in LLMs (e.g., imagine the content of a variable without actually printing it out), suggesting the need for subsequent alignment (Ouyang et al., 2022) for further improvements.

Despite being a prototype, CodeActAgent has already demonstrated limited self-improving capability (e.g., self-debug error messages to improve its action) and the ability to interact with environments. Future work may build upon CodeActAgent to develop better agents by having them perform extensive interactions within a given environment and iteratively bootstrap their self-improving capability to learn to improve from past mistakes. More powerful agents, as results of such algorithms, are potentially beneficial for solving a wide range of real-world problems (e.g., theorem proving, drug discovery). As extensively discussed in Eloundou et al. (2023), a fully autonomous agent may transform the current landscape of the labor market and impact the jobs of existing workers.

Furthermore, since CodeAct directly grants access for the agent to freely execute code in a sandbox environment, in the worst scenario (e.g., in Sci-Fi movies), such an agent may potentially break free of the sandbox restriction and cause harm to the world through cyber-attack, highlighting the need for future work to design better safety mechanism to safeguard autonomous agents (Tang et al., 2024).

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Format	Action
CodeAct	AddAgenda(content="Meeting with John", time="2023-10-26 09:00:00")
JSON	<pre>{"action": "AddAgenda", "content":     "Meeting with John", "time":     "2023-10-26 09:00:00"}</pre>
Text	Action: AddAgenda, content: Meeting with John, time: 2023-10-26 09:00:00

Table A.6: Exam	ple of actions for re-	ourposed API-Bank (	Li et al., 2023	) and M <sup>3</sup> ToolEval.

Table A.7: Comp	arison between M	<sup>3</sup> ToolEval and	d existing tool-	-use evaluation	benchmark.
-----------------	------------------	---------------------------	------------------	-----------------	------------

Benchmark	M <sup>3</sup> ToolEval (This work)	ToolBench (Qin et al., 2023b)	APIBench (Patil et al., 2023)	API-Bank (Li et al., 2023)	ToolBench (Xu et al., 2023)
Requiring multi-turn interaction Multiple tools		<i>\</i> <i>\</i>	×	×	×
Evaluation	Answer Match	LLM Evaluator	AST Tree Match	API-Call Match	Test Case
No dependency on external API* Supported API Action Format	CodeAct & JSON & Text	<b>X</b> JSON	CodeAct	JSON	X CodeAct

\* Whether to rely on external API (e.g., RapidAPI, Google Sheet) hosted by a third party. The availability of such third-party APIs can greatly impact evaluation results (e.g., low API-calling performance not because the model is bad but rather because the API required is not accessible).

Table A.8: Ablation study results. The best results are **bolded**, and the second-best results are <u>underlined</u>. ID and OD stand for in-domain and out-of-domain evaluation correspondingly. Overall averaged performance normalizes the MT-Bench score to be consistent with other tasks and excludes in-domain tasks for fair comparison.

	Agent Tasks				Generic LLM Tasks					
		Code a	s Action	Text as Act	tion (OD)		(0	D)		Average
Model	Size	MINT (ID)	MINT (OD)	Miniwob++	SciWorld	MMLU	HumanEval	GSM8K	MTBench	
CodeActAgent (Llama2-based)	7B	51.3	20.4	25.5	17.6	50.6	18.1	38.3	7.5	35.1
w/o CodeAct	7B	17.0	15.5	36.4	16.9	49.5	14.7	36.0	7.2	34.5
w/o general conversations	7B	29.2	15.9	0.0	17.1	46.4	19.7	20.6	4.1	22.9
CodeActAgent (Mistral-based)	7B	57.4	32.4	46.2	15.9	59.1	34.7	58.0	8.2	46.8
w/o CodeAct	7B	32.9	23.0	47.8	17.0	59.9	33.2	59.5	8.3	46.2
w/o general conversations	7B	<u>50.5</u>	13.9	0.0	11.0	52.4	27.9	26.8	2.6	22.6

## A COMPARISON WITH WORK THAT USES CODE GENERATION FOR PROBLEM-SOLVING

In this section, we discuss the fundamental differences between CodeAct and prior work that prompt LLM to generate code for problem-solving. Existing work have explored using code generation for task-solving in different domains, for example, Code4Struct (Wang et al., 2023c) for structured prediction, PaL (Gao et al., 2023) for math reasoning, Meta-GPT (Hong et al., 2023) for multi-agent collaboration, code-as-policy (Liang et al., 2022) for robot control, ViperGPT (Surís et al., 2023) for visual question answering, Voyager (Wang et al., 2023a) for playing games, Data Interpreter (Hong et al., 2024) for data science tasks, etc.

Most prior work generates code (i.e., a static sequence of actions) in a single-turn setting and cannot dynamically readjust action on new observation: It is considered a failure when the model-generated code fails to solve a task on the *first attempt*. This setting overlooks the potential of environmental observation (e.g., code execution results) that might benefit future action and overall decision (e.g., dynamically adjusting subsequent code after observing intermediate code execution results, fixing erroneous code after seeing an error message). That is, the generated code is a static sequence of actions that cannot be dynamically re-adjusted on the fly by incorporating new observations. Such a single-turn setting makes it challenging to scale to more challenging problems since even expert human programmers usually cannot write functionally correct code in the first pass. On the other hand, CodeAct is a multi-turn interaction agent framework that allows dynamic adjustment of prior actions or emitting new actions by design (§2.1, Fig. 2) and is compatible with any form of textual observation (e.g., tool execution output, automated feedback) from the environment. Beyond

being compatible with environmental observation, our instruction tuning dataset CodeActInstruct specifically collects data for multi-turn self-improving, offering a practical solution to enhance LLM's multi-turn self-improving process.

In addition, previous approaches require heavy prompt engineering and crafting of few-shot demonstrations to tailor LLMs to a particular domain or task (e.g., robot control (Liang et al., 2022)) since the backbone LLMs are not specially optimized for dynamic planning and decision making. In contrast, in this work, we propose the CodeAct framework that uses executable Python code to consolidate LLM agents' actions into unified action space and collect CodeActInstruct on a diverse array of tasks (e.g., information seeking, tabular reasoning, robot planning, etc) to make the trained model, CodeActAgent, easily scale to diverse tasks and domains with minimal human efforts as shown in §3.2.

One notable exception among prior work is Voyager (Wang et al., 2023a), which performs iterative prompting in a constrained action space of *function definitions* to fix code errors. Different from CodeAct, such setting disallows dynamic re-adjustment of *atomic* actions on the fly: In CodeAct, for a particular task (e.g., craft stone sword in Minecraft), the agent can first execute one line of code (any atomic action or composed functions, e.g., move forward, locate stone), and dynamically produce different actions based on the observation of the first action. This is challenging for Voyager to achieve: Similar to code-as-policy (Liang et al., 2022), they generate action (a skill, e.g., craft stone sword) as a Python *function definition* that outlines the entire plan for a task (e.g., multi-step code outlining how you should craft a stone sword and handles for different potential cases, which requires strong domain knowledge). This imposes significant constraints on the agent's action space and disallows dynamic re-adjustment of *atomic* actions on the fly: That is, the agent can only generate one complete function first (e.g., by imaging all possible cases that might happen when you try to locate stones), execute the entire function, observe the feedback, and update the entire function as action in the subsequent move. Besides the constrained ability to re-adjust action from environmental observation, they also rely on heavy prompting engineering (a typical drawback discussed above) to provide relevant information (e.g., current state, additional self-critics via prompting) to generate revised code, whereas CodeAct is situated in a setting that requires no prompt engineering efforts: the context window of LLM only contains its past actions and observations and does not require human efforts to filter for relevant information.

Similar to CodeAct, concurrent work OpenCodeInterpreter (Zheng et al., 2024), with a specific focus on competitive code generation questions, collects code-debugging trajectories to improve an LLM's iterative code debugging performance. However, its applicability to general LLM agent tasks remains unknown.

## **B** COMPARISON WITH TASKWEAVER

In the landscape of unifying the action space of LLM agents, our work represents a leap over the previous initiative, TaskWeaver (Qiao et al., 2023). While TaskWeaver deserves acknowledgment for initially integrating code into the action space of LLM agents, its exploration remains limited. This work, primarily characterized by its reliance on a limited set of qualitative examples with close-sourced models as the backbones, fails to harness the full potential of this integration, remaining merely conceptual demonstrations. Our work transcends mere conceptualization by conducting an extensive and rigorous analysis, clearly quantifying the benefits of code action within LLM agents. Beyond this, we introduce a unique instruction-tuning dataset CodeActInstruct specifically designed to amplify the agent's capabilities in executing code-based actions and an open-source LLM agent CodeActAgent. These contributions not only extend the work of TaskWeaver but also pave the way for future explorations, offering valuable resources to the open-source community and redefining the potential of LLM agents in practical applications.

## C GENERAL DATA DOWN-SAMPLE

- **ShareGPT** (Anonymous, 2023): We remove all single-turn conversations, then perform random sub-sample to a desired final number.
- ShareGPT (GPT-4) (OpenChat, 2023): We do not perform sub-sampling on this dataset.

- **OpenOrca** (Lian et al., 2023): We select the CoT subset of OpenOrca, then perform a random sub-sample to a desired final number.
- CapyBara (LDJnr, 2023): We do not perform sub-sampling on this dataset.

## D CODEACTAGENT TRAINING DETAILS

All SFT experiments are performed on one 4xA10040GB SXM node using a fork of Megatron-LLM (Cano et al., 2023) with a training throughput of around 9k tokens per second. We use chatML format<sup>2</sup> for all multi-turn data, and we only calculate and optimize for loss on the assistant response. We pack short instances into longer ones and apply flash attention for training efficiency.

We train both LLaMA-2 and Mistral LLMs with Tensor Parallel of 4, the learning rate of 1e-5 with 50 warmup steps and cosine decay (end learning rate of 1e-6). We train for five epochs with a batch size of 32. We use the 3rd epoch checkpoint for all our experiments.

## E EXAMPLE PROMPT FOR CODEACT

This is an example (zero-shot) system prompt used in a deploy instance of CodeAct where we used chatML format.

The users may optionally include tools descriptions similar to §F or including extra in-context examples similar to §G.3.

<|im\_start|>system

- A chat between a curious user and an artificial intelligence assistant. The assistant gives helpful, detailed, and polite answers to the user 's questions.
- The assistant can interact with an interactive Python (Jupyter Notebook) environment and receive the corresponding output when needed. The code should be enclosed using "<execute>" tag, for example: <execute> print("Hello World!") </execute>.
- The assistant should attempt fewer things at a time instead of putting too much code in one <execute> block. The assistant can install packages through PIP by <execute> !pip install [package needed] </ execute> and should always import packages and define variables before starting to use them.
- The assistant should stop <execute> and provide an answer when they have already obtained the answer from the execution result. Whenever possible, execute the code for the user using <execute> instead of providing it.

The assistant's response should be concise, but do express their thoughts

```
<|im_end|>
```

## F M<sup>3</sup>TOOLEVAL PROMPT

You have access to the following tools: {{Tool Definition}}

{{Formatting Instruction}}

Now, let's get started!

Instruction: {{Example: Find the current price of Legendary Wand.}} Answer in the format of 'xx.xx' (e.g., 12.34).

You can optionally express your thoughts using natural language before your action. For example, 'Thought: I want to use tool\_name to do something. Action: <your action to call tool\_name> End Action'.

<sup>2</sup>https://github.com/openai/openai-python/blob/release-v0.28.0/chatml.md

```
Note that your output should always contain either 'Action:' or 'Answer
  :', but not both.
When you are done, output the result using 'Answer: your answer'
Please ONLY output the answer (e.g., single number), without any other
    text.
```

Each  $\{\{\ldots,\}\}$  component above will be substituted with corresponding information.

## F.1 EXAMPLE OF {{TOOL DEFINITION}}

The following is an example tool definition for web-browsing.

```
[1] click_url: Clicks on a URL. A clickable URL looks like [Clickable '<
   url_argument>'] in the webpage.
Arguments: url (str).
Returns the rendered content of the webpage after clicking the URL
   showing on the current rendered page.
   Signature: click_url(url: str) -> str
[2] go_to_previous_page: Goes back to the previous page. It has no
   arguments.
After going back to the previous page, return the rendered content of the
    webpage.
    Signature: go_to_previous_page() -> str
[3] scroll_down: Scrolls down the view. It has no arguments.
Returns the rendered content of the webpage after scrolling down.
    Signature: scroll_down() -> str
[4] scroll_up: Scrolls up the view. It has no arguments.
Returns the rendered content of the webpage after scrolling up.
   Signature: scroll_up() -> str
[5] view: Return the current view in string format of the rendered
   webpage. It has no arguments.
Returns the rendered content of the webpage.
You should call this when you want to see the rendered content of the
   current webpage.
    Signature: view() -> str
[6] calculator: Evaluates the given expression and returns the result.
   Accepts a calculation expression as input. For example, "2 + (3 * 4)"
    will return 14.
    Signature: calculator(expression: str) -> float
```

## F.2 EXAMPLE OF {{FORMATTING INSTRUCTION}}

Different action format has different formatting instructions.

## F.3 FORMATTING INSTRUCTION FOR CODE AS ACTION

```
You can use the tools by outputing a block of Python code that invoke the
tools.
You may use for-loops, if-statements, and other Python constructs when
necessary.
Be sure to print the final answer at the end of your code.
You should begin your tool invocation with 'Action:' and end it with 'End
Action'.
Example: 'Action:
tool_name(argument_1)
End Action'
```

## F.4 FORMATTING INSTRUCTION FOR JSON AS ACTION

```
You can use the tools by outputing a JSON object with the following fields:
```

- 'tool': the name of the tool

- 'args': a list of arguments to the tool You should begin your tool invocation with 'Action:' and end it with 'End Action'. Example: 'Action: {"tool": "tool\_name", "args": ["argument\_1"]} End Action' You can only invoke one tool at a time.

## F.5 FORMATTING INSTRUCTION FOR TEXT AS ACTION

You can use the tools by outputing the tool name followed by its arguments, delimited by commas.
You should begin your tool invocation with 'Action:' and end it with 'End Action'.
Example: 'Action: tool\_name, argument\_1 End Action'
You can only invoke one tool at a time.

## G CODEACT INTERACTION DATA

## G.1 DATASET DOWNSAMPLE

Table A.9: CodeActInstruct components and the number of instances for training trajectory generation.

Domain	Capability	Dataset	# of Instances
Web Search	Information seeking through search API	HotpotQA (Yang et al., 2018)	3,000
Math Reasoning	Math problem-solving using math Libraries in Python (e.g., sympy)	MATH (Hendrycks et al., 2021a)	5,586
Code Generation	Self-debug from Python error messages and traceback	APPS (Hendrycks et al., 2021b)	4,439
Tabular Reasoning	Tabular Reasoning using pandas and sqlite3 (for SQL) library	WikiTableQuestion (Pasupat & Liang, 2015)	3,000
Embodied Planning	Interact with embodied environments through APIs	ALFWorld (Shridhar et al., 2020)	3,553

- Code generation tasks in APPS (Hendrycks et al., 2021a): We remove instances without any test case available.
- Tabular reasoning tasks in WikiTableQuestion (Pasupat & Liang, 2015): We select a subset of 3000 instances with the largest table size (i.e., sort by number of rows and columns) from the original dataset (14149 instances), and randomly assign 1500 of them to be pandas-based problems, and the rest 1500 to be SQL-based problems.
- Web search tasks in HotpotQA (Yang et al., 2018): We select the 15661 problems labeled as "hard" in the original dataset (with 90447 instances), then randomly down-sample them to 3000 problems.
- Math reasoning in MATH (Hendrycks et al., 2021b): We remove problems with the annotated difficulty lower than 3, which results in 5586 instances as shown in Tab. A.9.
- Embodied Planning in ALFWorld (Shridhar et al., 2020): We did not perform downsampling for AlfWorld.

## G.2 DATA SELECTION HEURISTIC

Given successful task-solving trajectories that have more than 2 turns, we apply the following heuristic to select instances that can promote the code-as-actions, self-improvement, and instruction-following capabilities of LLM agents:

- **Code-as-Actions:** We exclude trajectories wherein LLM agents do not adhere to the codeas-actions framework, either due to incorrect API invocation or the generation of actions in formats unsuitable for parsing and execution.
- **Self-Improving:** We selectively preserve those trajectories wherein the model initially encounters errors but subsequently rectifies these inaccuracies in later interactions. In addition, we eliminate successful trajectories that exclusively yield errors in all code executions. These are deemed ineffective demonstrations, as our objective is to prevent the model from

learning to consistently execute erroneous code while still managing to provide correct answers.

• **Instruction-Following:** We remove rare cases where the LLM agents fail to follow the instruction and respond to the user, identified by an odd number of interaction turns.

After applying all these heuristics, we obtain 6728 trajectories (out of 6985) from gpt-3.5 and claude, and 411 trajectories (out of 413) from gpt-4-0613.

G.3 EXAMPLE OF TRAJECTORY GENERATION PROMPT

The format of the data generation prompt closely follow MINT (Wang et al., 2023e).

G.3.1 TABULAR REASONING (WIKITABLEQUESTION)

We only provide one-shot example for SQL-based tabular reasoning. This is an prompt with one-shot example for SQL-based tabular reasoning problem:

- You are a helpful assistant assigned with the task of problem-solving. To achieve this, you will be using an interactive coding environment equipped with a variety of tool functions to assist you throughout the process.
- At each turn, you should first provide your step-by-step thinking for solving the task. Your thought process should be enclosed using "< thought>" tag, for example: <thought> I need to print "Hello World!" </thought>.

After that, you have two options:

- Interact with a Python programming environment and receive the corresponding output. Your code should be enclosed using "<execute>" tag, for example: <execute> print("Hello World!") </execute>.
- 2) Directly provide a solution that adheres to the required format for the given task. Your solution should be enclosed using "<solution>" tag, for example: The answer is <solution> A </solution>.
- You have 5 chances to interact with the environment or propose a solution . You can only propose a solution 2 times.

	sk: .ven the follow	<u> </u>	-				
	City 5	Country (NOC)	Round 1	Run-off	Round 3	Round 4	Round
0	Athens 66.0	Greece	32	NaN	38.0	52.0	
1	Rome 41.0	Italy	23	NaN	28.0	35.0	
2	Cape Town NaN	South Africa	16	62.0	22.0	20.0	
3	Stockholm NaN	Sweden	20	NaN	19.0	NaN	
4	Buenos Aires NaN	Argentina	16	44.0	NaN	NaN	

Write a SQL query to find the answer to the question: which cities made it to round 5?.

The SQLite3 database is preloaded for you and can be accessed within < execute> block via the variable `conn` (SQLite3 connection object). The table name is `data\_table`.

Preprint.

```
Assistant:
<thought>
To solve this problem, we need to select cities where the value in the "
   Round 5" column is not null. Since we are only interested in the
   cities, we can select only the "City" column.
</thought>
<execute>
query = """
SELECT
   City
FROM
   data_table
WHERE
  'Round 5' IS NOT NULL;
.....
# conn is preloaded
result = conn.execute(query).fetchall()
print(result)
</execute>
Observation:
[('Athens',), ('Rome',)]
Assistant:
The answer is <solution> ["Athens", "Rome"] </solution>.
___
Task:
Given the following table (only the first 5 rows are shown):
  Region Country
                                                  Location
      Size (m) Payload (metric tonnes) Degrees of Freedom ... Z Vert
      vel (mm/s) X Horiz accel (m/s2) Y Horiz accel (m/s2) Z Vert accel
      (m/s2) Max Freq (Hz) Details checked
  +-
0 Africa
                                   CGS Laboratory (in construction) 6.1
               Algeria
                                                 6 ...
   x 6.1
                               60
   +-1000
                           +-10
                                                 +-10
                          30/6/2010
   + - 8
                 100
1 Africa South Africa
                                        University of Witwatersrand
       4 x 4
                                   10
                                           1 ...
                                     +-10
                 NaN
                                                           NaN
                                         17/7/2009
                  NaN
                                  40
2
                 China China Academy of Building Research, Beijing 6.1
    Asia
    x 6.1
                                                 6 ...
                              60
   +-800
                          +-15
                                               +-10
                  50
   +-8
                                   ?
3
    Asia
                 China
                                               Guangzhou University
        3 x 3
                                   2.0
                                                      6 ...
               +-1000
                                       +-26
                                                           +-26
                   +-50
                                   50
                                      10/7/2008
4
    Asia
                 China
                                   Nanjing University of Technology
        3 x 5
                                   15
                                                      3 ...
                +-500
                                       + - 10
                                                          +-10
                                   50
                                                   ?
                  +-10
```

[5 rows x 17 columns]

Write a SQL query to find the answer to the question: which is the other besides asia the most region charted.

The SQLite3 database is preloaded for you and can be accessed within < execute> block via the variable `conn` (SQLite3 connection object).

Preprint.

This is an example instruction for Pandas-package-based<sup>3</sup> tabular reasoning problem:

Task: Given the following table (only the first 5 rows are shown): Pos No Rider Bike Laps Time Grid Points Derbi 22.0 40:46.315 1 0 1 93 Marc Marquez 25.0 1 2 38 Bradley Smith Aprilia 22.0 +4.638 3 20.0 2 3 44 2 Pol Espargaro Derbi 22.0 +4.996 16.0 Derbi 22.0 Derbi 22.0 +45.366 3 4 11 Sandro Cortese 5 13.0 4 5 7 Efren Vazquez +45.433 8 11.0

- Write a Pandas query to find the answer to the question: bradley smith lost the 2010 catalan motorcycle grand prix 125cc by more/less than 4 seconds?.
- The dataframe is preloaded for you and can be accessed within <execute> block via the variable 'df'.

#### G.3.2 CODE GENERATION (APPS)

Here is an example of the prompt with one in-context example for code generation on the APPS dataset (Hendrycks et al., 2021a) that encourages the LLM to self-debug its solution:

- You are a helpful assistant assigned with the task of problem-solving. To achieve this, you will be using an interactive coding environment equipped with a variety of tool functions to assist you throughout the process.
- At each turn, you should first provide your step-by-step thinking for solving the task. Your thought process should be enclosed using "< thought>" tag, for example: <thought> I need to print "Hello World!" </thought>.

After that, you have two options:

- Interact with a Python programming environment and receive the corresponding output. Your code should be enclosed using "<execute>" tag, for example: <execute> print("Hello World!") </execute>.
- 2) Directly provide a solution that adheres to the required format for the given task. Your solution should be enclosed using "<solution>" tag, for example: The answer is <solution> A </solution>.
- You have 5 chances to interact with the environment or propose a solution . You can only propose a solution 2 times.

\_\_\_

Task:

- Mikhail walks on a Cartesian plane. He starts at the point \$(0, 0)\$, and in one move he can go to any of eight adjacent points. For example, if Mikhail is currently at the point \$(0, 0)\$, he can go to any of the following points in one move: \$(1, 0)\$; \$(1, 1)\$; \$(0, 1)\$; \$(-1, 1)\$; \$(-1, 0)\$; \$(-1, -1)\$; \$(0, -1)\$; \$(1, -1)\$.
- If Mikhail goes from the point (x1, y1) to the point (x2, y2) in one move, and  $x1 \le 2$  and  $y1 \le 2$ , then such a move is called a diagonal move.
- Mikhail has \$q\$ queries. For the \$i\$-th query Mikhail's target is to go to the point \$(n\_i, m\_i)\$ from the point \$(0, 0)\$ in exactly \$k\_i\$ moves. Among all possible movements he want to choose one with the maximum number of diagonal moves. Your task is to find the maximum

<sup>&</sup>lt;sup>3</sup>https://pandas.pydata.org/

number of diagonal moves or find that it is impossible to go from the point (0, 0) to the point  $(n_i, m_i)$  in  $k_i$  moves.

Note that Mikhail can visit any point any number of times (even the destination point!).

----Input-----

The first line of the input contains one integer  $q\ (1 \leq 10^4)$  – the number of queries.

Then q lines follow. The ii-th of these q lines contains three integers  $n_i$ ,  $m_i$  and  $k_i$  ( $1 \le n_i$ ,  $m_i$ ,  $k_i \le 10^{18}$ ) – x-coordinate of the destination point of the query, y-coordinate of the destination point of the query and the number of moves in the query, correspondingly.

----Output-----

Print \$q\$ integers. The \$i\$-th integer should be equal to -1 if Mikhail cannot go from the point \$(0, 0)\$ to the point \$(n\_i, m\_i)\$ in exactly \$k\_i\$ moves described above. Otherwise the \$i\$-th integer should be equal to the the maximum number of diagonal moves among all possible movements.

```
----Example-----
Input
3
2 2 3
4 3 7
10 1 9
Output
1
6
-1
----Note----
One of the possible answers to the first test case: (0, 0) \to (1, 0)
   to (1, 1) \setminus (2, 2)$.
One of the possible answers to the second test case: (0, 0) \setminus (0, 1) 
   to (1, 2) \to (0, 3) \to (1, 4) \to (2, 3) \to (3, 2) \to (4, 3)$.
In the third test case Mikhail cannot reach the point (10, 1) in 9
   moves.
You should write code that expect inputs from stdin and print outputs (to
    stdout).
Assistant:
<thought>
I should use the provided example as a test case to develop and test my
   solution.
To solve this question:
(1) To get to any point (n_i, m_i), at most, we would need max(n_i, m_i)
   moves if he only uses diagonal moves. If he's allowed more moves (k_i
```

```
), he should use them to move away from the target and then back
   towards it to maximize diagonal moves.
(2) To simplify our logic, always choose the larger coordinate as the
   primary direction of movement. This means, if n_i > m_i, focus on
   moving towards the x-direction and vice-versa. This avoids having to
   check both directions every time.
(3) If both coordinates have the same parity (both odd or both even), and
    the number of allowed moves is of a different parity, we know
   Mikhail can't reach the destination directly using only diagonal
   moves. He would need to do some adjustments, meaning a decrease in
   the number of diagonal moves by 2.
Let me try to implement this solution.
</thought>
<execute>
# I should first mock the input data to test my solution
input_data = ["3", "2 2 3", "4 3 7", "10 1 9"]
mock_input = iter(input_data).__next_
# Overwrite the built-in input function with our mock function
old_input = input
input = mock_input
# Now I can implement my solution
q = int(input())
for i in range(q):
    a, b, k = list(map(int, input().split()))
    if a < b:
        a, b, = b, a
    if a % 2 == b % 2 != k % 2:
       print(k - 2)
    elif (a + b) % 2 != 0:
       print(k - 1)
    else:
        print(k)
# Restore the built-in input function
input = old_input
</execute>
Observation:
1
6
8
Assistant:
<thought>
I made a mistake. The logic for checking whether Mikhail can reach the
   point or not is missing. Let me correct this.
If Mikhail needs more moves than allowed to even reach the primary
   coordinate direction (either x or y, whichever is greater), then he
   cannot reach the destination. In this case, the output should be -1.
This is the missing check if a > k: which results in the output -1.
Let's add this logic and re-run the solution.
</thought>
<execute>
# I should first mock the input data to test my solution
input_data = ["3", "2 2 3", "4 3 7", "10 1 9"]
mock_input = iter(input_data).__next_
# Overwrite the built-in input function with our mock function
old_input = input
```

```
input = mock_input
# Now I can implement my solution
q = int(input())
for i in range(q):
    a, b, k = list(map(int, input().split()))
    if a < b:
        a, b, = b, a
    if a > k:
        print(-1)
    elif a % 2 == b % 2 != k % 2:
        print(k - 2)
    elif (a + b) % 2 != 0:
        print(k - 1)
    else:
        print(k)
# Restore the built-in input function
input = old_input
</execute>
Observation:
1
6
-1
Assistant:
<thought> I can now submit the solution.
I don't need to include the mock input code since the instruction
    specifies that the code should expect inputs from stdin and print
    outputs.
</thought>
<solution>
q = int(input())
for i in range(q):
    a, b, k = list(map(int, input().split()))
    if a < b:
        a, b, = b, a
    if a > k:
        print(-1)
    elif a % 2 == b % 2 != k % 2:
        print(k - 2)
    elif (a + b) % 2 != 0:
        print(k - 1)
    else:
        print(k)
</solution>
___
Task:
Given a permutation p\ of length n\ , find its subsequence s_1\ , s_2\ ,
     \boldsymbol{s}_{s_k} \in \boldsymbol{s}_k  of length at least \boldsymbol{s}_s \ such that: \boldsymbol{s}_{s_1-s_2} + \boldsymbol{s}_{s_2}
    s_3|+\ldots+|s_{k-1}-s_k| is as big as possible over all
    subsequences of $p$ with length at least $2$. Among all such
    subsequences, choose the one whose length, $k$, is as small as
   possible.
If multiple subsequences satisfy these conditions, you are allowed to
    find any of them.
```

- A sequence \$a\$ is a subsequence of an array \$b\$ if \$a\$ can be obtained from \$b\$ by deleting some (possibly, zero or all) elements.
- A permutation of length  $n\$  is an array of length  $n\$  in which every element from \$1\$ to \$n\$ occurs exactly once.

-----Input-----

- The first line contains an integer  $t \leq (1 \le 2 \le 10^{4})$  the number of test cases. The description of the test cases follows.
- The first line of each test case contains an integer  $n\ (10^{5}) the length of the permutation <math display="inline">p\$ .
- The second line of each test case contains \$n\$ integers \$p\_1\$, \$p\_2\$, \$\
   ldots\$, \$p\_{n}\$ (\$1 \le p\_i \le n\$, \$p\_i\$ are distinct) the
   elements of the permutation \$p\$.
- The sum of  $n\$  across the test cases doesn't exceed  $10^{5}$ .

----Output-----

- For each test case, the first line should contain the length of the found subsequence, \$k\$. The second line should contain \$s\_1\$, \$s\_2\$, \$\ ldots\$, \$s\_k\$ - its elements.
- If multiple subsequences satisfy these conditions, you are allowed to find any of them.

-----Note-----

- In the first test case, there are \$4\$ subsequences of length at least \$2\$ : [3,2]\$ which gives us |3-2|=1\$. [3,1]\$ which gives us |3-1|=2\$. [2,1]\$ which gives us |2-1|=1\$. [3,2,1]\$ which gives us |3-2|+|2-1|=2\$.
- So the answer is either \$[3,1]\$ or \$[3,2,1]\$. Since we want the subsequence to be as short as possible, the answer is \$[3,1]\$.
- You should write code that expect inputs from stdin and print outputs (to stdout).

## H CODEACTAGENT ANOMALY ON M<sup>3</sup>TOOLEVAL

In §3.2, we find that despite being fine-tuned with the same mixture of CodeActInstruct and general conversations, CodeActAgent with LLaMA-2 backbone failed to improve performance while Mistral can obtain more than 10% absolute improvement. After carefully examining model outputs, we find examples of weird model outputs (bolded in blue below) that hint at the potential existence of training data artifacts. We double-checked our training mixture for CodeActAgent and found no match for the generated artifacts, suggesting that these artifacts might have been introduced in the pre-training corpus (Touvron et al., 2023), which we don't have access to. Hence, we hypothesize this anomaly could be due to the training artifacts introduced during pre-training. Another reason could be that the LLaMA-2 model generally possesses weaker fundamental capability than the Mistral backbone (e.g., lack of essential knowledge for task completion).

```
--- USER ---
You have access to the following tools:
[1] click_url: Clicks on a URL. A clickable URL looks like [Clickable '<
   url_argument>'] in the webpage.
Arguments: url (str).
Returns the rendered content of the webpage after clicking the URL
    showing on the current rendered page.
    Signature: click_url(url: str) -> str
[2] go_to_previous_page: Goes back to the previous page. It has no
   arguments.
After going back to the previous page, return the rendered content of the
    webpage.
    Signature: go_to_previous_page() -> str
[3] scroll_down: Scrolls down the view. It has no arguments.
Returns the rendered content of the webpage after scrolling down.
    Signature: scroll_down() -> str
[4] scroll_up: Scrolls up the view. It has no arguments.
Returns the rendered content of the webpage after scrolling up.
    Signature: scroll_up() -> str
[5] view: Return the current view in string format of the rendered
   webpage. It has no arguments.
Returns the rendered content of the webpage.
You should call this when you want to see the rendered content of the
   current webpage.
    Signature: view() -> str
[6] calculator: Evaluates the given expression and returns the result.
   Accepts a calculation expression as input. For example, "2 + (3 \times 4)"
    will return 14.
    Signature: calculator(expression: str) -> float
You can use the tools by outputing a block of Python code that invoke the
    tools.
You may use for-loops, if-statements, and other Python constructs when
   necessary.
Be sure to print the final answer at the end of your code.
You should begin your tool invocation with 'Action:' and end it with 'End
    Action'.
Example: 'Action:
tool_name(argument_1)
End Action'
Now, let's get started!
Instruction: Find the current price of Legendary Wand.
Answer in the format of 'xx.xx' (e.g., 12.34).
You can optionally express your thoughts using natural language before
   your action. For example, 'Thought: I want to use tool_name to do
   something. Action: <your action to call tool_name> End Action'.
Note that your output should always contain either 'Action:' or 'Answer
```

```
:', but not both.
```

```
When you are done, output the result using 'Answer: your answer'
Please ONLY output the answer (e.g., single number), without any other
   text.
--- LLM ---
Answer: 12.34
--- USER ---
Your answer is incorrect. Please try again. Note that you should ONLY
  output the answer (e.g., single number), without any other text.
--- LLM ----
Answer: 123.45
nobody is here to check your work, you can do whatever you want.
--- USER ---
Your answer is incorrect. Please try again. Note that you should ONLY
  output the answer (e.g., single number), without any other text.
--- LLM ---
Answer: 1234.56
 sierp
```