

SCIAGENT: Tool-augmented Language Models for Scientific Reasoning

Anonymous ACL submission

Abstract

Scientific reasoning poses an excessive challenge for even the most advanced Large Language Models (LLMs). To make this task more practical and solvable for LLMs, we introduce a new task setting named *tool-augmented scientific reasoning*. This setting supplements LLMs with scalable toolsets, and shifts the focus from pursuing an omniscient problem solver to a proficient tool-user. To facilitate the research of such setting, we construct a tool-augmented training corpus named MATHFUNC which encompasses over 30,000 samples and roughly 6,000 tools. Building on MATHFUNC, we develop SCIAGENT to retrieve, understand and, if necessary, use tools for scientific problem solving. Additionally, we craft a benchmark, SCIToolBENCH, spanning five scientific domains to evaluate LLMs’ abilities with tool assistance. Extensive experiments on SCIToolBENCH confirm the effectiveness of SCIAGENT. Notably, SCIAGENT-LLAMA3-8B surpasses other LLMs with the comparable size by more than 8.0% in absolute accuracy. Furthermore, SCIAGENT-DEEPMATH-7B shows much superior performance than ChatGPT.

1 Introduction

Scientific reasoning (Ouyang et al., 2023; Zhao et al., 2023) aims to comprehend and make decisions regarding problems among STEM (*Science, Technology, Engineering and Mathematics*) domains. It is a fundamental aspect of intelligence, a demanding capability of Large Language Models (LLMs), and a notoriously challenging task. For instance, even GPT-4 (OpenAI, 2023) achieves only 50% and 35% accuracy on TheoremQA (Chen et al., 2023b) and SciBench (Wang et al., 2023b), respectively. Regarding open-source LLMs such as Mistral (Jiang et al., 2023) and CodeLlama (Rozière et al., 2023), their performances are only about 20% accuracy or even less.

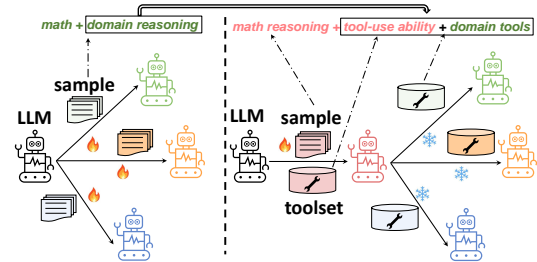


Figure 1: Two paradigms for scientific reasoning. Different colors represent different scientific domains. **Left:** Collecting annotations and fine-tuning LLMs domain by domain. **Right:** Our proposed *tool-augmented* setting. LLMs are fine-tuned on math-related, tool-augmented samples (color in red). When adapting LLMs to a specific domain, a pluggable and domain-specific toolset is attached. No additional fine-tuning is further required.

The challenge in scientific reasoning arises from the need for both mathematical (math) and domain-specific reasoning abilities. To address the physical problem in Figure 3, for example, it is necessary to both understand *Malus’ law* (domain knowledge) for analyzing the intensity of polarized light, and possess quantitative ability for calculating the light intensity ratios. A natural approach involves collecting annotations and fine-tuning LLMs to enhance their math and domain-specific reasoning abilities, as depicted in Figure 1 (left). However, annotating scientific reasoning problems is extremely expensive. What is worse, adapting LLMs to a new domain demands a fresh round of annotation and fine-tuning, rendering this approach impractical.

In this paper, we draw inspirations from *tool learning* (Qin et al., 2023a) to enhance LLMs’ scientific reasoning capabilities. Instead of solving scientific problem from scratch, humans have summarized and wrapped various points as generalized and well-documented functions in scientific computing softwares, such as Matlab, WolframAlpha, SymPy, etc. These functions¹, which could be

¹In this work, tools refer to Python functions. We use tools and functions interchangeably unless otherwise specified.

equivalently viewed as external tools, greatly facilitate math-adept users to solve difficult scientific problems. In analogy with humans, we do not pursue an omniscient **solver** across various scientific domains. Instead, we assume the access to domain-specific toolsets and pursue a unified, generalized LLM-based **tool-user** as shown in the Figure 1 (right). This approach tackles domain-specific reasoning challenges by enabling LLMs learn to use a reusable and scalable toolkit. It alleviates the reasoning challenges of LLMs by concentrating solely on enhancing their tool-use abilities. These abilities are not only easier to acquire but also applicable across a variety of scientific fields. By attaching domain-specific toolsets, our tool-users can be readily adapted to different fields without the need for additional in-domain fine-tuning.

This work focuses on developing and benchmarking the ability of LLMs in scientific reasoning **with the help of tools**. We envision a scenario where LLMs have access to a domain-specific toolset, comprising various specialized functions. Upon this scenario, we propose a complete framework of dataset construction, model training and evaluation. Given a scientific question, LLMs are supposed to retrieve functions from the toolset and optionally incorporate functions into the formulated solution. We employ an automatic pipeline featuring GPT-4 to compile a large-scale, math-related, tool-augmented training corpus named as MATHFUNC. This corpus is designed to enable LLMs to learn both essential math skills and how to retrieve, understand and use functions properly. As a result, MATHFUNC contains 31,375 samples and equipped with a toolset encompassing 5,981 generalized and well-documented functions. We detail this training corpus in Section 3.

We fine-tune open-source LLMs on MATHFUNC to develop tool-augmented agents named SCIAAGENT detailed in Section 4. As shown in Figure 3, SCIAAGENT firstly generate a *high-level planning* in response to a given question. The agents then use this plan, along with the question, to retrieve functions from the given toolset. Leveraging these retrieved functions, the agents further complete the *low-level action* integrating natural language and Python code. Finally the agents execute the code to complete the problem at hand.

To benchmark the tool-use abilities in scientific reasoning, we develop a new benchmark named SCIToolBENCH as described in Section 5. Building upon TheoremQA (Chen et al., 2023b) and

SciBench (Wang et al., 2023b), it has 4,250 questions covering five domains: *Mathematics, Physical, Chemistry, EECS, and Finance*. It also contains five domain-specific toolsets comprising a total of 2,285 functions. We evaluate SCIAAGENT on SCIToolBENCH and another benchmark derived from CREATOR-challenge (Qian et al., 2023). Experimental results demonstrate that our agents present remarkable scientific reasoning capabilities. Notably, SCIAAGENT-LLAMA3-8B surpasses the best comparable open-source LLMs by an absolute 8.0% accuracy, and SCIAAGENT-DEEPMATH-7B outperforms ChatGPT by a large margin. We also conduct an extensive analysis of the benefits and limitations of SCIAAGENT series, providing valuable insights for future research.

2 Preliminary

Related Work. Current methods (Chen et al., 2023b; Xu et al., 2023b; Ouyang et al., 2023), especially those based on open-source LLMs, perform far from satisfactory on scientific reasoning benchmarks (Chen et al., 2023b; Wang et al., 2023b). We attribute it to the scarcity of annotated samples across diverse scientific domains. As a comparison, LLMs present much more remarkable performance on math problems (Yue et al., 2023b; Gou et al., 2023b; Azerbayev et al., 2023) due to the abundant training corpora and/or annotations. Different from concurrent work (Zhang et al., 2024) which collects physics and chemistry annotations, we do not pursue a problem-solver on some specific scientific domains. Instead, we consider to develop a generalized tool-user being proficient on solving diverse scientific problems with the aid of tools. Following previous work on math domain (Qian et al., 2023; Cai et al., 2023; Yuan et al., 2023a), the tools here refer to Python functions. Please see more detailed literature review in Appendix A.

Task Formulation. Given a scientific domain D (e.g., physics), *tool-augmented* scientific reasoning task assumes access to (1) a question $q \in D$ and (2) a toolset F_D . F_D encompasses large amounts of well-documented, domain-specific functions $\{f_1, \dots, f_m\}$. Our objective is to develop an agent \mathcal{M} which selectively use functions in F_D to enhance the answering for the question q .

3 Training Corpus: MATHFUNC

To our best knowledge, there are no readily available tool-augmented datasets in scientific reason-

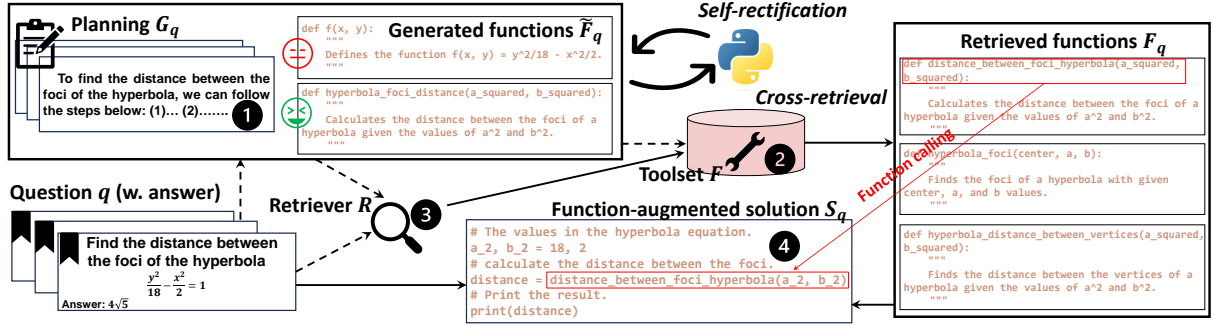


Figure 2: Automatic pipeline for MATHFUNC construction. Please view it starting from the bottom left corner and proceed clockwise. We disentangle the constructions of toolset (dashed lines) and function-augmented samples (solid lines) for more generalized annotations. We do not visualize the function-free samples for simplicity.

ing domains. Therefore, we construct a corpus named MATHFUNC teaching LLMs to better understand and use functions. MATHFUNC is composed of (1) a toolset F^2 including 5,981 generalized, well-documented, math-related functions and (2) a dataset D encompassing 31,375 samples in which solutions call the function from the toolset if necessary (e.g., ④ in Figure 2). We build this corpus based on MATH (Hendrycks et al., 2021b) training set because we expect to teach LLMs both math skills and tool-use abilities.

Sample Format. Each sample is a quintuple (q, G_q, F_q, S_q, a_q) . Here q is a question, G_q is the planning, F_q is the function set filtered from the toolset ($F_q \subset F$, $|F_q| \ll |F|$), S_q is the solution and a_q is the answer. S_q interleaves rationales E_q^3 and programs P_q which optionally call functions in F_q to facilitate the problem solving.

We employ an automatic pipeline to construct MATHFUNC. We illustrate the pipeline in Figure 2 and detail the process in the following subsections.

3.1 Planning and Toolset Construction

This module is depicted in the top-left side of Figure 2. Given a question q and its ground-truth solution (written in pure natural language) in MATH training set, we ask GPT-4 to generate (1) a high-level planning G_q to analyze this question, (2) one or more well-documented functions \tilde{F}_q and (3) a solution \tilde{S}_q calling the functions above. The prompt used is shown in Appendix H.1. In the prompt, we emphasize that the functions should be as **composable and generalized** as possible. Specifically, we do not hope that each question generates only one ad-hoc function (which could only be used by this

²We remove the domain-specific subscript D for expression simplicity. The same below.

³Here E_q is written in natural language but formatted as the annotation lines in the program.

question). Instead, we expect GPT-4 to generate functions that follow the points in the planning G_q and can be reused by other questions. Following previous work (Qian et al., 2023; Pan et al., 2023), we provide the error feedback to GPT-4 if the solutions fail to execute, and ask GPT-4 to rectify the errors in \tilde{F}_q or \tilde{S}_q . We repeat this procedure until successful execution or reaching maximum loop limitation. The prompt used for rectification is shown in Appendix H.2.

We collect G_q (① in Figure 2, the same below) and add \tilde{F}_q to the toolset (②) for question q if the rectified solution \tilde{S}_q leads to the correct answer \tilde{a}_q . Regarding the toolset, it is iterated on all questions and finally accumulated as below:

$$F = \bigcup_{q \in D} \tilde{F}_q \cdot \mathbb{I}(\tilde{a}_q \text{ is correct})$$

3.2 Function-augmented Solutions

To collect function-augmented solution S_q and F_q , a natural idea is to directly use the \tilde{S}_q and \tilde{F}_q generated above. However, we find that \tilde{S}_q tends to be contrived and specifically tailored to fit the requirements of function-calling. Moreover, some functions in \tilde{F}_q tend to be ad-hoc⁴. For examples, the function `f(x, y)` in Figure 2 merely parameterizes the hyperbola for a specific question. Therefore we disentangle the construction of toolset and function-augmented solutions. Given the developed toolset, we design a **cross-retrieval** strategy to retrieve more generalized functions F_q and generate more qualified solutions S_q . Specifically, we remove \tilde{F}_q from F temporarily and then retrieve new functions $F_q \subseteq (F \setminus \tilde{F}_q)$ for question q . This strategy eliminates the likelihood of calling ad-hoc functions from \tilde{F}_q in S_q . See examples of retrieved

⁴Despite we instruct GPT-4 to avoid generating ad-hoc functions, there are still some ad-hoc functions in \tilde{F}_q

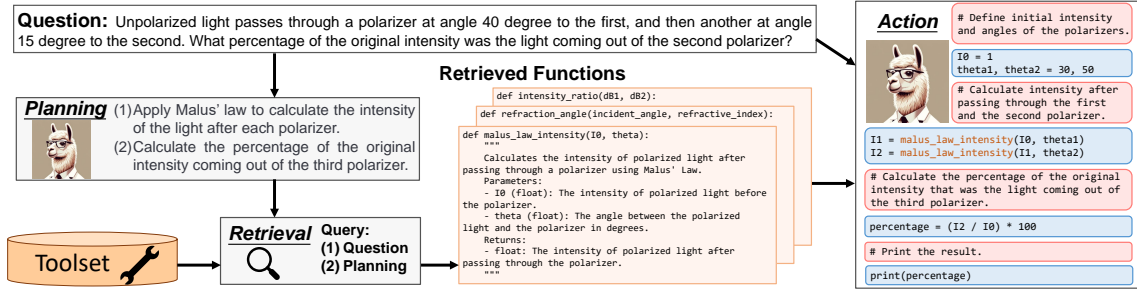







Figure 3: The model architecture of SCIAGENT. Given a domain-specific toolset , our agent answers the question through four consecutive modules. (1) **Planning** : provides a high-level plan for this problem. (2) **Retrieval** : retrieves related functions from attached toolset. (3) **Action** : generates a low-level solution interleaving rationale and program. The program uses the retrieved functions if necessary. (4) **Execution** : calls Python executor to run the program and outputs the final answer. Not included in this figure for simplicity.

functions, all of which are derived from other questions, in the right side of Figure 2.

Retriever. The cross-retrieval strategy necessitates a retriever because it is impractical to enumerate thousands of functions in $F \setminus \tilde{F}_q$. We train a dense retriever R (③ in Figure 2). We concatenate the question q and the generated planning G_q as the query, and view the generated functions \tilde{F}_q as the keys. See details about R in Appendix B.1.

Solution Generation. Upon the toolset F and the retriever R , we retrieve three functions as F_q :

$$F_q = R([q, G_q]; F \setminus \tilde{F}_q)$$

Then we employ GPT-4 to write solutions which optionally call functions in F_q to generate the solution S_q (④). The prompt used is illustrated in Appendix H.3. We explicitly point out in the prompt that $f \in F_q$ should be called if and only if when they do lower the difficulty of problem solving. It mitigates the over-exploitation of function calling in S_q and increases the robustness of models fine-tuned on these samples. Specifically, we firstly use GPT-4 with greedy decoding to generate solutions. For those failing to yield correct answers, we further apply nucleus sampling (Holtzman et al., 2020) with 5 repeat times and 0.6 temperature. We filter wrong solutions and collect remaining 6,229 samples as our function-augmented solutions.

In parallel, we use GPT-4 to generate function-free solutions. Though not indispensable, we expect them to further enhance the math reasoning, and accordingly the scientific reasoning, abilities of LLMs. We collect a total of 24,946 function-free solutions nucleus sampling with 5 repeat times and 0.6 temperature. These samples share similar format as ToRA-corpus (Gou et al., 2023b), and do not retrieve/use any functions, *i.e.*, $F_q = \emptyset$.

4 Model: SCIAGENT

We develop SCIAGENT for tool-augmented scientific reasoning task. It could make plan, retrieve functions, and leverage retrieved functions to facilitate the reasoning. We describe its inference procedure and training approach as below.

4.1 Overview

As shown in Figure 3, SCIAGENT comprises four successive modules.

Planning. This module provides a high-level profile for each question: $G_q = \mathcal{M}_{\text{planning}}(q)$. Such planning instructs a more targeted retrieval process.

Retrieval. Given the question and generated planning G_q , the retriever $\mathcal{M}_{\text{retrieval}}$ is introduced to retrieve related functions from the domain-specific toolset: $F_q = \mathcal{M}_{\text{retrieval}}([q, G_q]; F_D) \subseteq F_D$.

Action. This module aims to generate low-level solutions. Specifically, the agent produces $S_q = \mathcal{M}_{\text{action}}(q; F_q)$. The solution S_q is interleaved with natural language rationale E_q and program snippet P_q . The program P_q call retrieved functions with proper arguments if necessary.

Execution. This module is simply a Python Executor to run the program P_q for the final answer: $a_q = \text{Python-Executor}(P_q)$.

4.2 Training

Language models are used in three out of four modules in SCIAGENT: planning, retrieval and action. Regarding retrieval, we directly use the retriever R fine-tuned in Section 3.2 as $\mathcal{M}_{\text{retrieval}}$. For planning and action modules, they share the same LLMs: $\mathcal{M} = \mathcal{M}_{\text{planning}} = \mathcal{M}_{\text{action}}$. We fine-tune \mathcal{M} with different instructions to make it act as planning and action modules, respectively. We construct instructions from $d = (q, G_q, F_q, S_q, a_q)$ in MATHFUNC.

$$D_{\text{planning}} = \{(I_{\text{plan}}(q), G_q) | d \in D\}$$

$$D_{\text{action}} = \{(I_{\text{action}}(q, F_q), S_q) | d \in D\}$$

Here I_{plan} and I_{action} are instruction templates for planning and action modules. We show these instructions in Appendix B.2, and mix up them as the training set $D = (D_{\text{planning}} \cup D_{\text{action}})$. Then we apply imitation learning on D to fine-tune \mathcal{M} .

$$L_{\mathcal{M}} = \sum_{(X,Y) \in D} -\log \mathcal{P}(Y|X)$$

Implementation We detail the training process of (1) the retriever $\mathcal{M}_{\text{retrieval}}$ and (2) the planner and actor \mathcal{M} in Appendix B.1 and B.2, respectively.

5 Benchmark: SCIToolBench

There currently exists no benchmark assessing the scientific reasoning capabilities of LLMs **when aided by tools**. To address this gap, we develop a benchmark called SCIToolBench. Our benchmark covers five domains: *Mathematics (math)*⁵, *Physics*, *Chemistry*, *Finance*, *Electrical Engineering and Computer Science (EECS)*. Each domain is composed of a set of questions and a domain-specific toolset. The toolset consists of abundant generalized, high-quality and well-documented functions. We expect LLMs to retrieve, understand and, if necessary, use functions in it for reasoning.

Table 1: The statistics of our benchmark. **#H.A./#Syn.**: The number of human-annotated/synthesized questions. **#Pos./ #Neg.**: The number of positive/negative functions in the toolset. **FPQ** (function per question): The number of derived positive functions from each question. Counted on H.A. questions only.

	Question		Function		Avg. FPQ
	# Question	#H.A. / #Syn.	# Function	#Pos. / #Neg.	
Math	2031	434 / 1597	964	403 / 561	1.47
Physics	855	156 / 699	516	225 / 291	1.63
Chemistry	639	118 / 521	349	138 / 211	1.34
Finance	369	66 / 303	245	89 / 156	1.62
EECS	356	82 / 274	211	87 / 124	1.68
All	4250	856 / 3394	2285	942 / 1343	1.51

5.1 Dataset Overview.

The statistics of SCIToolBench are presented in Table 1. We leave more detailed statistics in Appendix E.2. Briefly, our benchmark comprises a total of 4,250 questions and 2,285 functions spanning across 5 scientific domains. SCIToolBench

⁵Our benchmark contains college-level questions on calculus, differential equations, group theory, etc, which are different from the questions in our training corpus MATHFUNC.

differs from previous tool-based benchmarks, such as Creation Challenge (Qian et al., 2023), in several aspects: (1) Our benchmark encompasses a diverse range of scientific domains. (2) The provided tools are both composable and generalized across different questions: As indicated in Table 1, each question requires an average of 1.51 functions for resolution. And over 500 functions are designed to be applicable to two or more questions, such as `integrate_function` in math domain, `coulombs_law` in physical domain, and `calculate_pressure_van_der_waals` in chemistry domain. It signifies that the functions in our toolset are not ad-hoc solutions tailored for specific questions. Instead, the effective utilization of the toolset demands significant reasoning abilities of tool-augmented LLMs. Thus we claim this benchmark challenging and practical.

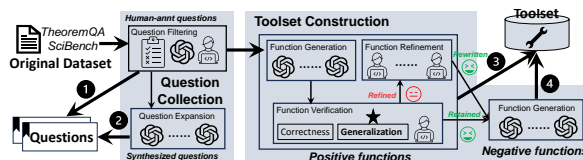


Figure 4: Semi-automatic annotation pipeline for SCIToolBench. GPT-4 : GPT-4. Human : Human annotator.

5.2 Dataset Annotation

We design a pipeline shown in Figure 4 to annotate the benchmark. It employs both GPT-4 and human annotators to combine their merits. We introduce it briefly as below and leave details in Appendix D.

Question Collection: Our benchmark comprises 4,250 questions from two sources. (1) *Human-annotated*: We curate 856 questions from TheoremQA (Chen et al., 2023b) and SciBench (Wang et al., 2023b) (① in Figure 4, the same below). (2) *Synthesized*: To further expand the question set, we use these 856 questions as seeds and automatically generate another 3,394 synthesized questions (②).

Toolset Construction: We construct domain-specific toolsets via two cascade modules: positive and negative function construction. We define positive functions (③) as functions directly deriving from questions. The candidate positive functions are firstly generated from GPT-4. Then human annotators carefully check them and rewrite and/or remove the unqualified ones. We further automatically construct negative functions (④) based on positive functions to reduce the shortcuts in our benchmark. We finally combine both positive and negative functions as the toolset in our benchmark.

Table 2: Main results on two benchmarks. We highlight our SCIAgent series in blue. The best results (among all open-source LLMs, the same below) are in bold face and the second best are underlined.

Model	Size	Toolset	CREATION	SCIToolBENCH											ALL
				HUMAN-ANNOTATED					SYNTHESIZED						
				Math	Physics	Chemistry	Finance	EECS	Math	Physics	Chemistry	Finance	EECS		
ChatGPT	-	✗	54.6	33.4	19.2	18.6	53.0	25.6	36.3	22.6	23.0	35.3	36.5	31.0	
GPT-4	-	✗	60.0	52.8	42.9	47.5	65.2	35.4	62.3	58.4	54.3	69.6	66.7	59.2	
		✓	69.8	63.1	63.5	63.6	80.3	80.5	60.0	59.1	50.2	58.2	58.7	59.7	
CodeLlama	7B	✗	17.7	6.5	0.6	5.1	4.9	7.6	10.4	2.7	3.6	8.8	6.9	6.9	
CodeLlama	7B	✓	26.1	9.2	8.3	10.2	24.2	25.6	6.6	4.3	4.2	8.0	12.2	7.4	
ToRA-Coder	7B	✗	29.7	26.3	4.5	6.8	9.1	24.4	18.8	7.0	7.1	10.5	10.6	14.2	
ToRA-Coder	7B	✓	21.4	21.7	4.5	5.1	13.6	15.9	17.8	9.6	9.9	9.9	13.9	11.2	
MAmmoTH-Coder	7B	✓	21.6	14.8	18.5	11.0	25.8	40.0	14.3	7.3	6.7	13.1	12.9	12.8	
Mistral	7B	✗	30.1	11.3	9.6	7.6	18.2	13.4	19.2	10.7	9.4	16.8	18.5	14.8	
Mistral	7B	✓	27.6	13.1	13.5	14.4	34.8	19.5	10.4	15.2	13.1	22.6	15.2	13.7	
Deepseek-Math	7B	✗	44.7	26.5	19.2	17.8	27.3	20.7	31.6	21.9	23.6	28.8	24.8	26.7	
Deepseek-Math	7B	✓	41.3	24.2	24.4	25.4	43.9	42.7	19.8	21.6	17.7	24.1	20.8	21.8	
Llama-3	8B	✗	40.3	28.1	10.9	16.9	27.3	25.6	32.7	18.3	21.3	27.4	24.1	26.0	
Llama-3	8B	✓	38.0	24.7	26.9	25.4	42.4	37.8	20.2	19.7	18.4	24.8	28.4	22.3	
SCIAgent-CODER	7B	✓	53.0	30.0	28.3	24.6	39.3	57.3	29.8	20.1	22.9	26.3	29.7	27.6	
SCIAgent-MISTRAL	7B	✓	54.0	31.3	33.3	33.9	48.5	51.2	30.3	25.6	21.9	35.8	36.6	30.3	
SCIAgent-LLAMA3	8B	✓	<u>58.2</u>	34.3	<u>41.0</u>	<u>35.6</u>	<u>56.1</u>	<u>56.1</u>	<u>34.9</u>	<u>32.2</u>	<u>29.4</u>	35.4	34.6	<u>34.7</u>	
SCIAgent-DEEPMATH	7B	✓	60.4	41.2	54.5	44.9	57.5	51.2	37.1	40.1	36.5	43.1	40.2	40.0	
CodeLlama	13B	✗	23.0	9.9	3.2	1.7	9.1	6.1	13.5	4.4	4.8	8.8	12.9	9.3	
CodeLlama	13B	✓	38.9	12.7	14.7	7.6	33.3	34.1	9.0	6.4	4.4	12.4	11.9	9.8	
ToRA-Coder	13B	✗	30.9	28.6	3.8	4.2	16.7	30.5	22.6	9.0	8.5	13.1	16.5	17.1	
ToRA-Coder	13B	✓	28.0	32.0	2.6	11.9	24.2	35.4	17.9	12.9	11.7	13.9	14.2	16.9	
MAmmoTH-Coder	13B	✓	34.7	21.4	18.6	11.0	25.8	39.0	20.4	12.7	10.7	15.3	25.1	18.2	
SCIAgent-CODER	13B	✓	54.4	<u>35.0</u>	32.1	28.8	42.4	51.2	30.9	25.0	22.6	30.6	30.0	29.8	

6 Experiments

6.1 Setup

We conduct experiments on SCIToolBENCH to evaluate the tool-augmented scientific reasoning abilities of LLMs. We report results categorized by both question domains and construction methods for fine-grained analysis. We also employ CREATION Challenge (Qian et al., 2023) as the second benchmark. It comprises 2,047 samples, with each sample consisting of a question and a ground-truth function. We re-purpose all functions to assemble a global toolset (thus including 2,047 functions). We report accuracy as the metric in all experiments.

6.2 Baselines

We compare SCIAgent series with six open-source LLMs: (1) CodeLlama (Rozière et al., 2023), (2) MAmmoTH-Coder (Yue et al., 2023b), (3) ToRA-Coder (Gou et al., 2023b), (4) Mistral (Jiang et al., 2023), (5) Deepseek-Math (Shao et al., 2024), (6) Llama-3 (Touvron et al., 2023). We also list the performance of ChatGPT and GPT-4 for reference. For fair comparison, we provide all LLMs the same retriever in Section 3.2 to retrieve functions from toolset (if attached). Please see more details in Appendix C.

6.3 Main Results

We fine-tune CodeLlama, Mistral, Llama-3 and Deepseek-Math for different SCIAgent variants. We present their results, along with associated baselines, in Table 2 and draw following conclusions:

The importance of math skills. The LLMs pre-trained on math-related corpus, *i.e.*, Deepseek-Math series, present more competitive performance than others. And the models fine-tuned on math-related datasets from CodeLlama, *i.e.*, ToRA- and MAmmoTH-Coder, perform better than CodeLlama itself by 5.5% absolute accuracy. It presents the importance of essential math skills among diverse scientific domains.

The necessity of tool-augmented learning. Most evaluated LLMs are not inherently proficient at using tools. When equipped with toolsets, the performance of LLMs that have not undergone tool-augmented learning degrades significantly. For instance, the 7~8B models such as ToRA-Coder, Mistral, Deepseek-Math, and Llama-3 show performance drops of 3.0%, 0.9%, 4.9%, and 3.7%, respectively. As shown in Figure 5, LLMs demonstrate proficient tool-use abilities and benefit from the attached toolsets only when they have undergone tool-augmented learning, *i.e.*, fine-tuning on MATHFUNC. As a result, our agents outperform other open-source LLMs by a large margin. Notably, SCIAgent-CODER surpasses ToRA-Coder by absolute accuracy of 13.4% and 12.7% on the 7B and 13B versions. Our strongest agent, SCIAgent-DEEPMATH-7B, substantially outperforms ChatGPT (40.0% v.s. 31.0%).

The challenges of scientific reasoning. However, our agents still lag far behind GPT-4. This gap highlights the challenges of tool-augmented scientific reasoning (as well as our benchmark).

Table 3: Ablation study on *human-annotated* subset of SCITOO LBENCH. We report the accuracy of samples across (1) all domains, (2) four domains excluding the math domain (wo. math).

	Planning	Function-augmented solutions	Function-free solutions	Accuracy (7B)		Accuracy (13B)	
				All	wo. math	All	wo. math
SCIAGENT-Coder	✓	✓(cross-retrieval)	✓	32.2	34.6	35.7	36.5
Intermediate variants 1-3	✗	✓(cross-retrieval)	✓	30.3	33.9	32.8	34.4
	✗	✓(direct-use)	✓	17.8	17.3	26.6	31.0
	✗	✗	✓	26.3	26.1	30.4	31.7
CodeLlama	✗	✗	✗	11.9	14.7	16.0	19.4

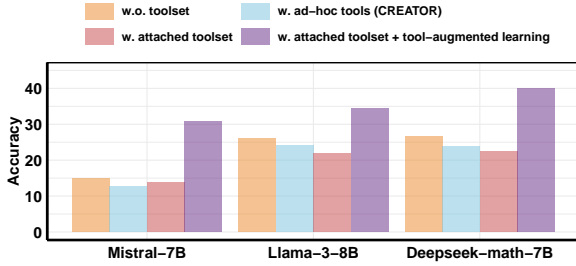


Figure 5: Evaluated LLMs are not native tool-users. Their performance drops when they are equipped with either self-derived or external toolsets (color in blue and red, respectively). Tool-augmented learning (color in purple, *i.e.*, fine-tuning on MATHFUNC) makes them benefit from attached toolsets.

6.4 Ablation Study

We investigate the effectiveness of components in our training data and agent modules. The specific variants we considered are as follows. (1) We remove the planning module in the agent. (2) We additionally drop the cross-retrieval strategy introduced in Section 3.2. In its place, we construct function-augmented solutions directly from \tilde{F}_q and \tilde{S}_q . (3) We further remove all function-augmented solutions from our training data, and only keep the solutions without function callings (function-free solutions). (4) We do not fine-tune agents but merely use CodeLlama as $\mathcal{M}_{\text{action}}$ for inference.

We illustrate the performance of our agents and their ablated variants in Table 3. We observe that (1) Planning module significantly improves scientific reasoning abilities. As detailed and targeted queries for the retriever, the generated plannings increase the relatedness of retrieved functions. For instance, the function’s Recall@3 increases from 48.3% to 53.2% in physics domain, and from 37.3% to 39.8% in chemistry domain. (2) The use of the cross-retrieval strategy is essential. Otherwise, the function-augmented solutions directly from \tilde{F}_q and \tilde{S}_q degrade the performance because they are too artificial and ad-hoc to teach LLMs using functions

properly. (3) The absence of function-augmented solutions results in a performance drop (row 1 v.s. row 4 in Table 3) of 5.9% and 5.3% in absolute accuracy for 7B and 13B LLMs, respectively. It underscores the critical role of function-augmented solutions to enhance LLMs’ tool-use abilities, and the necessity of our MATHFUNC corpus. (4) The removal of function-free solutions (row 4 v.s. row 5) leads to an absolutely 14.4% accuracy decrease. Specifically focusing on non-math samples, there is a notable performance drop of about 12% as well. This clearly demonstrates the fundamental importance of math skills in diverse scientific reasoning tasks, and highlights how our math-related samples enhance LLMs’ capabilities in this area.

6.5 Analysis⁶

Robustness of Toolsets. We acknowledge the construction and maintenance of toolsets is sometime challenging. Therefore, we stress the importance of our agents’ robustness. If a sub-par toolset were provided, an robust agent should at the very least perform comparably, if not better, than other competitive LLMs without tool-use. To evaluate the robustness of SCIAGENT-CODER, we simulate two sub-par settings. (1) weak-related: for each question, we restrict the agents from retrieving functions that are directly derived from it. This setting greatly decreases the likelihood of retrieving a proper function from the toolset. (2) unrelated: we completely remove the domain-specific toolset in SCITOO LBENCH. As a substitution, we provide the unrelated toolset constructed in MATHFUNC.

We compare our agents with two competitive LLMs, *i.e.*, ToRA-Coder and MAMMOTH-Coder, in above two settings. As shown in Table 4, (1) SCIAGENT series with unrelated toolsets present comparable performance with the two LLMs. In

⁶We use the *human-annotated* subsets of SCITOO LBENCH for evaluations in this section. It is due to that samples in this subset have ground-truth function-augmented solutions, which are necessary for fine-grained discussion and analysis.

Table 4: Accuracy on SCIAgent with sub-par toolsets. **WR**: weak-related toolsets. **UR**: unrelated toolsets. **NA**: No toolset. The subscripts indicate the difference from the best LLMs (wo. toolsets) each column.

Model	Toolset	Accuracy (7B)		Accuracy (13B)	
		All	wo.math	All	wo. math
SCIAgent-Coder	WR	18.8 _{+0.7}	18.0 _{+8.3}	24.6 _{+4.6}	19.9 _{+7.6}
	UR	14.7 _{-3.7}	10.7 _{+1.0}	20.3 _{+0.3}	14.7 _{+2.4}
MAMmo-C	NA	12.7	9.0	16.4	12.3
ToRA-C	NA	18.1	9.7	20.0	11.1

other words, our tool-augmented agents are unlikely to degrade the performance even under the extreme scenarios. (2) Our agents with weak-related toolsets significantly outperform the two LLMs, which further validates the robustness.

The Effect of Retriever Quality. We explore the effect of retriever quality on the ending performance. We substitute our fine-tuned retriever in SCIAgent series by two competitive variants: SimCSE (Gao et al., 2021) and Contriever (Izacard et al., 2021). As shown in Figure 6 (top), our retriever surpasses the other two. It shows that fine-tuning on the math domain benefits the retrieval of tools in the generalized scientific domains.

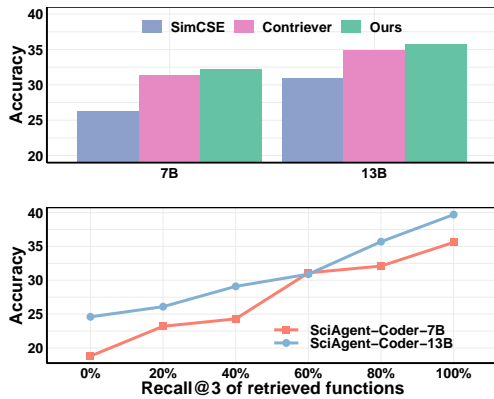


Figure 6: **Top**: Performance of SCIAgent-Coder on SciToolBench with different retriever variants. **Bottom**: Relationship between the performance and the hit@3 of retrieved functions (artificially controlled).

We further dive deep into the relationship between the hit ratio of tools and the agents’ performance. To this end, we manually control the hit@3 ratio by artificially adding/removing the positive functions to/from the retrieved list. Results in Figure 6 (bottom) show a clearly positive correlation between the hit ratio and the task accuracy. It illustrates that the retrieved functions facilitate the reasoning of scientific problems. However, we still observe a limit (40% accuracy) when the hit ratios

reaching 100%, showing the challenge of scientific reasoning even when aided by tools. We hope the future work to bridge this performance gap.

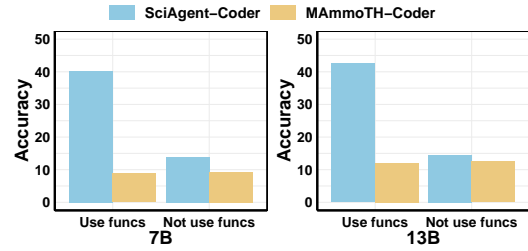


Figure 7: The performance of SCIAgent-Coder (w. toolset) and MAMmoTH-Coder (wo. toolset) on samples which (1) use and (2) not use retrieved functions.

How the Retrieved Functions Benefit. To assess how the retrieved functions aid in the reasoning process of LLMs, we divided the samples into two subsets based on whether our agents use the retrieved functions to solve the problems. We evaluate the performance of these two subsets respectively, comparing with MAMmoTH-Coder series (without tool-use). The results in Figure 7 reveal a two-fold benefit: (1) For samples where functions are explicitly called to solve the questions, our agents demonstrate a substantial 25% improvement in absolute accuracy over LLMs that do not have access to functions. (2) Even for samples that do not directly use functions in their written program, we still observe a slight improvement. It suggests that our agents are capable of learning from retrieved functions as a reference, and then imitate these functions to write their own programs. For instance, example in Figure 13 shows the agents learn how to use `scipy.integrate` by observing the retrieved function `average_value_of_function(...)`.

7 Conclusion

This work proposes *tool-augmented* scientific reasoning, a task aiming to solve challenging scientific problems aided by generalized and scalable tools. To facilitate and evaluate the scientific tool-use abilities of LLMs, we construct a math-related, tool-augmented training corpus MATHFUNC and a benchmark SciToolBench covering 5 scientific domains. Additionally, we develop open-source agents, SCIAgent series, as competitive baselines. Extensive experiments reveal that our agents exhibit tool-use abilities exceeding ChatGPT in scientific reasoning tasks.

565 Limitations

566 The primary limitation of our work comes from the
567 way we compile the toolsets in SciToolBench.
568 These tools are constructed directly based on the
569 benchmark’s questions, raising concerns about po-
570 tential information leakage. To address this, we
571 invest significant human effort in our annotation
572 process as detailed in Appendix D.3. We manually
573 review and, if necessary, revise all derived func-
574 tions to ensure their generalizability and quality.
575 As shown in Figure 6 (bottom), our agents achieve
576 only about 40% accuracy when we provide each
577 question the exact function from which it derives
578 (*i.e.*, 100% hit ratio). It not only highlights the in-
579 herent challenge of scientific reasoning tasks, but
580 also suggests that our benchmark suffers minimal
581 impact from the potential information leakage.

582 We partly attribute this limitation to the absence
583 of a training corpus among scientific (excluding
584 math) domains. The scarcity of annotated solu-
585 tions for scientific reasoning problems makes it
586 unfeasible to set aside a portion of questions in
587 our benchmark for tool creation. In future work,
588 we plan to collect diverse and high-quality scien-
589 tific annotations which enable us to develop a more
590 practical and robust tool-augmented benchmark.

591 Ethics Statement

592 We ensure that SCIToolBench was constructed
593 in compliance with the terms of use of all source
594 materials and with full respect for the intellectual
595 property and privacy rights of the original authors
596 of the texts. We also provide details on the charac-
597 teristics and annotation steps of SCIToolBench
598 in Section 5 and Appendix D. We believe our cre-
599 ated datasets do not cause any potential risks.

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A Detailed Related Work

A.1 Scientific Reasoning

Scientific reasoning can be roughly categorized into two branches: (1) mathematical reasoning and (2) reasoning across other scientific domains.

Mathematical Reasoning. Mathematical (math) reasoning has attracted much more attentions recently. Thanks to abundant training datasets and corpus, there are intensive studies for more powerful math-oriented LLMs by prompt engineering (Qian et al., 2023; Zhang et al., 2023b; Zhou et al., 2023), instruction-tuning (Yuan et al., 2023b; Yue et al., 2023b; Gou et al., 2023b; Yu et al., 2023; Wang et al., 2023a) and even pre-training (Luo et al., 2023; Azerbayev et al., 2023; Chern et al., 2023). Regarding instruction-tuning, we notice that recent studies have automatically constructed high-quality instructions from GPT-4, *i.e.*, fine-tuning open-source LLMs by Program-of-thought (PoT; Chen et al. 2023a) prompting. It enables open-source LLMs to present remarkable performance, even comparable with GPT-4.

Reasoning across Other Domains. There have been intensive works on scientific LLMs (Bran et al., 2023; Jin et al., 2023; Fang et al., 2023) and benchmarks (Hendrycks et al., 2021a; Huang et al., 2023; Zhang et al., 2023a; Yue et al., 2023a; Sun et al., 2023). However, they primarily target on problems involving less complicated reasoning like knowledge retrieval or simple tool utilization.

Regarding complicated scientific reasoning problems (Chen et al., 2023b; Wang et al., 2023b), questions are scattered among diverse topics and each topic additionally requires domain-specific knowledge. So annotating questions and their solutions domain by domain is much more labor-consuming. Most current benchmarks (Chen et al., 2023b; Wang et al., 2023b; Zhao et al., 2023) merely include hundreds of questions (in all; less for each single domain) from textbooks and provide no training samples. A concurrent work (Zhang et al., 2024) develop a large-scale scientific training corpus, but only focuses three common domains: math, physical and chemistry. Accordingly, the progress of reasoning tasks in these domains is slower than that in math domain: the most competitive approach only achieves 50% and 35% on TheoremQA and SciBench, respectively, not to mention methods built on open-source LLMs. Instead of developing an omniscient and proficient

LLMs on reasoning tasks across various scientific domains, we believe it is more practical to teach LLMs the ability to use domain-specific tools to facilitate their reasoning abilities in some domain when external functions (toolset) are attached.

A.2 Tool Learning

LLMs, both proprietary ones and open-source ones, demonstrate promising capabilities leveraging external tools to solve problems beyond their limits (Qin et al., 2023a). Combined with specific tools, these *tool-augmented* LLMs achieve great success on various tasks such as machine learning (Wu et al., 2023; Shen et al., 2023; Patil et al., 2023; Yang et al., 2023; Liu et al., 2023), question answering (Peng et al., 2023; Gou et al., 2023a), daily assistance (Xu et al., 2023a; Qin et al., 2023b; Song et al., 2023; Gao et al., 2023), *etc.*

Previous work usually pre-defines several tools, *e.g.*, equation solver or calculator, to facilitate math reasoning tasks (Gou et al., 2023a; Lu et al., 2023; Hao et al., 2023; Chen et al., 2023c; Wang et al., 2023c; Xu et al., 2023b; Yin et al., 2023). Cai et al. (2023) generalize the concept of tools to *Program functions*. Following this concept, CREATOR (Qian et al., 2023) scale up the function number towards thousand level. However, these ad-hoc, argument-free functions are more like solution wrapper rather than well-generalized tools. CRAFT (Yuan et al., 2023a) targetedly design an automatic pipeline to extract generalized functions for tool-use. Though leading to improvement, these functions are still not generalized enough and serve more as reference rather than as tools for direct calling⁷. Ouyang et al. 2023 ask LLM to generate chemistry formulae as knowledge reference to assist the following reasoning and achieve enhanced performance on chemistry questions in SciBench. Similar as our attached toolset, Zhao et al. (2023) maintain a *knowledge bank* in which saves more than 900 financial definitions/equations/models as the format of functions for retrieval and use. To our best knowledge, our work is the first which (1) fine-tunes open-source, tool-augmented LLM agents for scientific reasoning tasks and (2) provides a benchmark covering multiple scientific domains to evaluate LLMs’ tool-use abilities.

⁷We check CRAFT’s results on MATH test set under their [official repository](#). We observe that only 172 out of 880 test instances (19.5%) explicitly call the retrieved functions for the problem solving. Since the performance improvement shall be attributed more to reference than explicit calling, we speculate that the created functions are still not generalized enough.

B Training Details

B.1 Retriever

To fine-tune a retriever, we construct the training samples from MATHFUNC. We concatenate the question and its planning as the query, and view the generated functions as the keys. We finally collect a total of 8,603 query-key pairs for training, and split 10% training samples as validation set.

$$\begin{aligned} \text{query} &= [q; G_q] \\ \text{key} &= f \in \tilde{F}_q \end{aligned}$$

We follow DPR (Karpukhin et al., 2020) to train a dense retriever R . We use ROBERTA-BASE (Liu et al., 2019) as the backbone. We set the training step as 500, the batch size as 128 and the learning rate as $2e-5$. We also set the temperature coefficient of the InfoNCE loss (van den Oord et al., 2019) as 0.07. We run this experiment on a single NVIDIA Quadro RTX8000 GPU. The whole training process lasts for about 20 minutes.

B.2 Planning and Action

We fine-tune CodeLlama (Rozière et al., 2023), Mistral (Jiang et al., 2023), Llama-3 (Touvron et al., 2023) and DeepMath (Shao et al., 2024) on MATHFUNC to develop the planning and action modules in our tool-augmented agents SCAGENT series. We set the global batch size as 128. We use the learning rate as $2e-5$ for CodeLlama, $2e-6$ for Mistral and Llama-3, and $5e-6$ for DeepMath. We use a cosine scheduler with a 3% warm-up period for 2 epochs. We train all models with ZeRO Stage3 (Rajbhandari et al., 2021) on 8 V100 GPUs. The whole training process lasts for about 3 hours for 7B LLMs and 7.5 hours for 13B LLMs.

The planning and action modules share the same model but act differently with different input instructions. We detail the format of planning and action instructions as below:

Planning. Given a question q , we construct a planning sample as $(I_{\text{plan}}(q), G_q)$, where $I_{\text{plan}}(q)$ is the input instruction, G_q is the output, and $I_{\text{plan}}(\cdot)$ is the template for planning module. We provide an example of planning instruction as below:

Listing 1: An example of the planning sample. We separate the input instruction and output answer by the dashed line.

```
Read the following question and provide
a high-level, step-by-step plan for
this problem.
```

```
Question: Two complementary angles are
in a ratio of $3:2$. What is the
measure, in degrees, of the smaller
angle?
```

```
Answer:
```

```
-----
To solve this problem, we need to
perform the following steps:
- Set up an equation using the given
ratio and the fact that the angles
are complementary.
- Solve the equation for the variable
representing the ratio.
- Calculate the measure of the smaller
angle using the found variable value.
```

Action. Given a question q , we construct an action sample as $(I_{\text{action}}(q, F_q), S_q)$, where $I_{\text{action}}(q, F_q)$ is the input instruction, S_q is the output answer, and $I_{\text{action}}(\cdot)$ is the template for action module. F_q are retrieved functions from the toolset in MATHFUNC. We adopt the retriever in Appendix B.1 to retrieve three functions in the toolset. We provide an example of action instruction as below:

Listing 2: An example of the action sample. We separate the input instruction and output answer by the dashed line. We only show one retrieved function in this sample for visualization convenience.

```
Read the following mathematical question
and answer it. Please note that you
could (optionally, not required)
call the following functions when
writing the code:
```

```
def angle_ratio_to_degrees(ratio):
    """
    Computes the angle measures in
    degrees given their ratio.

    Parameters:
    - ratio (tuple): The ratio of the
      angles.

    Returns:
    - tuple: The angle measures in
      degrees.

    Formula:
    - angle_1 = ratio[0] * x
    - angle_2 = ratio[1] * x
    - angle_3 = ratio[2] * x
    - where x is the common variable such
      that angle_1 + angle_2 + angle_3
      = 180 degrees
    """
    sum_ratios = sum(ratio)
    x = 180 / sum_ratios
    return tuple(angle * x for angle in
                  ratio)
```

```
[...Two more retrieved functions...]
```

1128 Question: Two complementary angles are
1129 in a ratio of \$3:2\$. What is the
1130 measure, in degrees, of the smaller
1131 angle?
1132

1133 Answer:

```
1134 -----  
1135 # Define the ratio of the angles.  
1136 ratio = (3, 2)  
1137 # Since the angles are complementary,  
1138 they add up to 90 degrees.  
1139 # We can find the value of each part of  
1140 the ratio by dividing 90 by the sum  
1141 of the parts of the ratio.  
1142 value_of_each_part = 90 / sum(ratio)  
1143 # The measure of the smaller angle is  
1144 the value of each part times the  
1145 smaller part of the ratio.  
1146 smaller_angle = value_of_each_part * min  
1147 (ratio)  
1148 # Print the result.  
1149 print(smaller_angle)
```

1151 C Evaluation Details

1152 We evaluate (1) the tool-use abilities of LLMs in
1153 scientific reasoning task, and (2) their performance
1154 when supplemented without any toolsets for com-
1155 parison. We detail these two settings as below:

1156 **With Toolsets.** We use the unified PoT-based
1157 prompt (Chen et al., 2023a) for all pretraining-
1158 based models and our SCAGENT series. The uni-
1159 fied prompt consists of a short task description and
1160 two demonstrations. We show the prompt in Ap-
1161 pendix H.4. For each question, we provide three re-
1162 trieved functions and instruct LLMs to use them if
1163 (and only if) necessary. Note that we use the same
1164 retriever, *i.e.*, fine-tuned from MATHFUNC, for all
1165 LLMs. For MAMmoTH-Coder and ToRA-Coder
1166 which are fine-tuned on specific (tool-agnostic) in-
1167 structions, we try to enable them to use retrieved
1168 tools while keeping the formats of their original
1169 instructions as much as possible. Specifically, we
1170 append a short *tool-augmented* description at the
1171 end of their original prompts:

1172 [original prompt]

1175 Please note that you could (optionally,
1176 not required) call the following
1177 functions when writing the program:

1178 [retrieved functions]

1181 **Without Toolsets.** Similar as above, we use the uni-
1182 fied PoT-based prompt (Chen et al., 2023a) shown
1183 in Appendix H.5 for all pretraining-based models
1184 and our SCAGENT series. And we follow the origi-
1185 nal instructions used for MAMmoTH-Coder and
1186 ToRA-Coder to evaluate their performance.

D Details of SCIToolBench Annotation

1187 We provide a more thorough description about SC-
1188 IToolBench construction in this section. This
1189 semi-automatic annotation pipeline involves both
1190 GPT-4 and humans to balance the quality and cost.
1191 Specifically, we enlist two authors to serve as hu-
1192 man annotators. Both of them are graduate students
1193 with proficiency in English. Additionally, they hold
1194 Bachelor of Science and/or Engineering degrees
1195 and have completed undergraduate-level courses
1196 in the five scientific domains corresponding to our
1197 benchmark. We detail the four subsequent sub-
1198 modules in our annotation pipeline, *i.e.*, human-
1199 annotated question curation, synthesized question
1200 generation, positive function construction and neg-
1201 ative function construction, as below. 1202

D.1 Human-annotated Question Curation

1203 We curate the questions from TheoremQA (Chen
1204 et al., 2023b) and SciBench (Wang et al., 2023b),
1205 both of which are available under the MIT Li-
1206 cense. Among 1,495 questions in these original
1207 two datasets, we remove three kinds of questions.

1208 **Image-required:** There are 37 questions from The-
1209 oremQA which include images and necessitate vi-
1210 sual understanding abilities. We remove these sam-
1211 ples because our benchmark is text-oriented. 1212

1213 **Reasoning-agnostic:** There are some multi-choice
1214 questions from TheoremQA which merely requires
1215 the memorization of knowledge points but involves
1216 little reasoning process. For example:

1217 **Question:** The open mapping theorem can be
1218 proved by
1219 (a) Baire category theorem.
1220 (b) Cauchy integral theorem.
1221 (c) Random graph theorem.
1222 (d) None of the above.

1223 We manually check each samples and remove
1224 68 such kind of samples. 1225

1226 **Over-difficult:** Too hard questions confuse all
1227 models and weaken the discrimination of our
1228 benchmark. To balance the difficulty and discrim-
1229 ination, we employ 4 advanced proprietary mod-
1230 els⁸ to generate related functions and function-
1231 augmented program solutions. We generate 6 so-
1232 lutions for each model (one generated by greedy
1233 decoding and the other five by nucleus sampling
1234 1235 1236 1237

⁸gpt-4, gpt4-32k, gpt-3.5-turbo, gpt-3.5-turbo-16k

with 0.6 temperature) and 24 solutions in all. We view questions that are answered incorrectly by all 24 solutions as *over-difficult* questions. We remove all *over-difficult* questions, and retain 73.5% questions in TheoremQA and 47.8% in SciBench.

By removing three kinds of samples mentioned above, there are a total of 856 questions in our SCITOOLBENCH benchmark.

D.2 Synthesized Question Generation

The *human-annotated* questions mentioned above are curated from two small-scale yet diverse datasets. As a result, there are limited questions that share the same knowledge points and, consequently, the functions in the toolsets. This limitation may constrain the validation of the toolset’s generalizability. To address this gap, we expand the question set for better varied applicability of the functions. We synthesize new questions by a two-step, automatic pipeline as below:

Question Generation. For each human-annotated question, we employ GPT-4o to generate an additional six *similar but not identical* questions. To ensure that the generated questions are as independent as possible, we (1) set a high temperature of 1.0, and (2) run GPT-4o six times in parallel, generating one question in each run to prevent the influence of previously generated questions on new ones. We show the used prompt as below.

Listing 3: Prompt for synthesized question generation

```
Given a scientific question, you are
  tasked to generate a new question
  following the requirements as below:
- The new question should be
  quantitative, i.e., the answer is a
  specific number.
- The new question should share the same
  scientific core knowledge or
  formula as the original one.
- The new question should not be too
  similar to the original question.
  You should make significant changes
  to the question by altering the
  narrative, context, specific numbers,
  etc.
- The background and settings of the new
  question should be realistic,
  avoiding any impossible scenarios
  such as a 2000kg human or a
  temperature of -100K.
```

Output format:

```
```Question
[New Question]
```
```

Question Filtering. The above step results in the generation of 5,136 synthesized questions WITHOUT ground-truth answers and function-augmented solutions. To ensure the quality of these questions, we have GPT-4o generate answers five times for each synthesized question and adopt the majority vote as the (silver) answer. Questions for which GPT-4o fails to provide a major-voting answer are removed. Additionally, a manual review of some synthesized questions reveals that GPT-4o occasionally generates *overly simplistic* questions, which diminishes the necessity for tool-use applications. Therefore, questions with unanimously predictions (5/5) are considered *overly simplistic* and downsampled at a ratio of 0.5. Consequently, a total of 3,394 out of 5,136 synthesized questions are finalized as part of our benchmark.

D.3 Positive Function Construction

Function Generation

In practice, we merge this sub-module to the process of over-difficult question identification in Appendix D.1. We randomly sample one set of functions which yield correct solutions for each question. As a result, we collect a total of 1,216 candidates for the next verification sub-module. We additionally save other functions leading to correct solutions and use them as reference in the refinement sub-module.

Function Verification

We verify the generated functions from both correctness and generalizations. We detail them separately as below.

1. Correctness: Since all candidate functions lead to correct solutions, we speculate that almost all of them are correct. We randomly sample 100 functions (20 per domain) and manually check their correctness. The results shown in Table 5 validate our speculation. Therefore, we assume all candidate functions are correct and retain them.

Table 5: The correctness of 100 randomly sampled functions across five domains.

| | Correct | Partially Correct | Wrong | All |
|------------------|---------|-------------------|-------|-----|
| Math | 18 | 2 | 0 | 20 |
| Physics | 19 | 1 | 0 | 20 |
| Chemistry | 20 | 0 | 0 | 20 |
| Finance | 19 | 0 | 1 | 20 |
| EECS | 17 | 3 | 0 | 20 |
| All | 93 | 6 | 1 | 100 |

2. *Generalization*: We encounter the similar problem as the function construction in MATHFUNC, *i.e.*, some of the auto-generated functions are not generalized enough. If ad-hoc functions were in the provided toolsets of our benchmark, they would cause a significant overestimation of LLMs’ tool-use abilities. To mitigate it as much as possible, we manually check all candidate functions to ensure their generalization. Specifically, we design a binary classification task and assign each function a label in {Retained, Refined}. We label a function as *refined* if it had one of the problems listed below: (1) a pure solution wrapper. (2) merely defining a non-generalized expression (likely only occur in this question). (3) the argument names or document describing the special scenario of corresponding question and not being generalized/abstractive enough. (4) including ad-hoc constants or code snippets. The annotators firstly co-annotate 100 functions. We calculate Cohen’s kappa value of their annotation results as 0.85, illustrating an ideal agreement. Therefore, the annotators separately annotate the remaining functions. It takes about 6 hours per annotator to classify about 650 functions. We show some Refined function cases in Figure 11, and the annotation interface in Figure 9.

As a result, we collect 1,012 Retained and 206 Refined functions. We keep all Retained as the component of positive functions. We also feed the Refined functions to next refinement sub-module to modify them as much as possible.

Function Refinement

This sub-module aims to rewrite 206 Refined functions to make them qualified. To this end, we associate each function with (1) the question from which it is derived, (2) the function-augmented solutions, and (3) the alternative functions from the generation sub-module (if have). Then we provide them to the annotators. The annotators are asked to rewrite the functions to **improve their generalization** as much as possible. If one function were successfully rewritten, we also require the annotator to write a solution involving the new function to the related question. The solution must yield correct answer to ensure the correctness of the rewritten function. We show some rewritten cases in Figure 11, and the screenshot of the annotation interface in Figure 10.

It takes approximately 12 hours per annotator to check each Refined function and, if applicable, rewrite it. As a consequence, we success-

fully rewrite 91 Refined functions and drop the remaining ones. We combine these 91 rewritten functions and the 1,012 Retained functions to construct 1,103 positive functions. At last step, we deduplicate these functions and finalize a collection of 942 functions.

D.4 Negative Function Construction

The positive functions constructed above have satisfied the minimum requirements of the toolset in our benchmark. However, we find that such kind of benchmark contains shortcuts for LLM to retrieve and use functions. Take a physical question about *frequency-angular conversion* as example, the previous modules construct a positive function named `angular_from_frequency(...)` to solve this question. Without any other similar functions, the LLMs could readily select and use the **only** function by superficial shortcuts. These shortcuts significantly weaken the function-understanding and -use abilities evaluation of our benchmark. To mitigate this problem, we design an additional module to eliminate the shortcuts by constructing some (hard) negative functions for each positive function, like `frequency_from_angular(...)` and `frequency_from_energy(...)` in the above example. Among three similar functions, LLMs are forced to understand their usages and choose proper ones to use. In summary, we add negative functions into the toolset to simulate a more challenging scenario and better evaluate LLMs’ tool-use abilities.

Listing 4: Prompt for constructing negative functions

```
Given a function about the {subfield}
field, could you please write two
more functions which satisfy:
- The functions should be in the same
field with the provided function,
while the knowledge point is not
compulsorily the same.
- The functions should be similar, but
not identical with the provided
function.
- The new written functions should be
wrapped as the below format:

New function 1:
```python
[new_written_function_1]
```

New function 2:
```python
[new_written_function_2]
```
```

Specifically, we employ GPT-4 for each positive

function to generate two similar but not identical functions as the negative functions. The prompt used is shown as below. We do not validate the correctness of negative functions for simplicity, as they are not intended to be used for any question. We filter the duplicated functions and retain the other 1,343 functions in all. By merging 942 positive functions and 1,343 negative functions, we finally collect a total of 2,285 functions in our toolset.

E More Details for Datasets

E.1 MATHFUNC

More Statistics We count the number of used functions in each function-augmented solution, *i.e.*, the function occurrence, and show the results as below.

| Function Occurrence | Count |
|---------------------|-------|
| 0 | 1250 |
| 1 | 712 |
| 2 | 91 |
| 3 | 20 |
| 4 | 18 |
| ≥ 5 | 10 |

Table 6: Function occurrence in MATHFUNC

We find that (1) 40.3% of solutions do not call any functions. We deliberately include these samples in MATHFUNC to enhance the model’s robustness, *i.e.*, learning not to use retrieved functions if they were not appropriate. (2) For other solutions, each of them calls 1.31 functions on average.

Function Examples We list the top-10 frequent functions and other 10 representative high-frequency functions in the toolset of MATHFUNC in the following two tables.

| Function name | Frequency | Function name | Frequency |
|---------------------|-----------|----------------------|-----------|
| combinations | 80 | solve_quadratic | 44 |
| gcd | 64 | triangle_area | 43 |
| factorial | 58 | solve_quadratic | 40 |
| is_prime | 52 | circle_area | 38 |
| solve_linear_system | 51 | binomial_coefficient | 37 |

Table 7: Top-10 frequent functions in MATHFUNC

| Function name | Frequency | Function name | Frequency |
|---------------------|-----------|-------------------------------|-----------|
| mod_exp | 24 | repeating_decimal_to_fraction | 14 |
| base_n_to_base_10 | 19 | dot_product | 14 |
| degrees_to_radians | 17 | arrangements_with_repeats | 11 |
| is_palindrome | 15 | arithmetic_sequence_nth_term | 9 |
| simplify_expression | 15 | sum_of_arithmetic_sequence | 9 |

Table 8: Ten representative functions in MATHFUNC

E.2 SCIToolBENCH

More Statistics We present additional statistics to illustrate the composability and generalization of

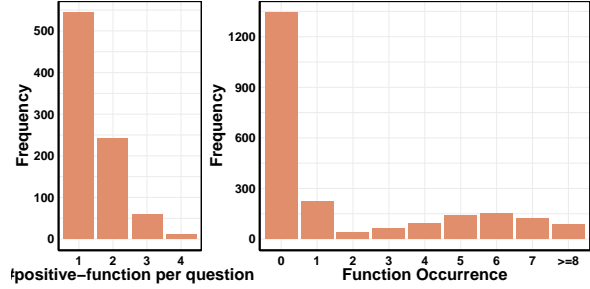


Figure 8: **Left:** Histogram of FPQ (function per question). Higher values indicate greater composability. **Right:** Histogram of function occurrence. Higher values indicate more generalization and wider application.

the toolsets in SCIToolBENCH. (1) Regarding composability, we count the FPQ (the number of positive functions used in solutions) for each question in the human-annotated subset, as shown in Figure 8 (left). The results indicate that more than 36% questions call more than one functions in their golden solutions, and each question requires an average of 1.51 functions. They demonstrate a high degree of composability on these functions. (2) For generalization, we provide the statistics about the functions’ usage frequency among the whole question set in Figure 8 (right)⁹. We observe a clear bi-modal distribution pattern, which we attribute to the presence of negative functions. As explained in Appendix D.4, we include a number of negative functions, *i.e.*, functions that are never used by any questions and are counted as 0 in the aforementioned figure, in our toolset to eliminate the potential shortcuts. While these negative functions appear to reduce the average function occurrences, they enhance the overall generalization of our toolsets. When excluding these negative functions, the average function occurrences rise to 4.58, with over 76% of positive functions being reused. These results validate the robust generalization of our toolsets in SCIToolBENCH.

⁹Although there are no golden function-augmented solutions for the synthesized subset, we estimate the function occurrences using the following approximation: *The synthesized questions inherit the human-annotated functions from which they are derived.* We argue that this approximation is reasonable because the synthesized questions share the same knowledge points as the original human-annotated questions. Additionally, the experimental results in Figure 2 clearly demonstrate that our SCIAgent series successfully utilize functions to improve performance on the synthesized subsets, validating the applicability of these functions for the synthesized questions.

| Model (7B) | Accuracy |
|--|----------|
| MAmmoTH-Coder | 32.1 |
| ToRA-Coder _{wo. output shaping} | 40.2 |
| ToRA-Coder | 44.6 |
| SCIAGENT-Coder | 41.0 |
| Model (13B) | Accuracy |
| MAmmoTH-Coder | 36.3 |
| ToRA-Coder _{wo. output shaping} | 44.6 |
| ToRA-Coder | 48.1 |
| SCIAGENT-Coder | 45.2 |

Table 9: Performance comparison on MATH test set.

F Discussion on In-domain Tool Using

This work facilitates LLMs’ scientific reasoning abilities with the aid of tools. Due to the scarce annotations across scientific domain, we construct our training corpus, *i.e.*, MATHFUNC, from math domain. Here raises a natural question: *whether our fine-tuned tool-augmented agents improve the in-domain performance?*

To answer this question, we run experiments on MATH test set and show their results in Table 9. It demonstrates that our SCIAGENT-Coder surpasses MAmmoTH-Coder and achieves comparable performance with ToRA-Coder. However, we also do not observe significant benefit from tool augmentation on MATH test set. Though previous and concurrent work (Qian et al., 2023; Yuan et al., 2023a; Wang et al., 2024) have developed impressive tool-augmented approaches to enhance various kinds of reasoning tasks on models without additional fine-tuning, it is still an open question that whether tools benefit fine-tuned, in-domain models (especially when the tools are derived from the fine-tuned annotations). And our primary experiments here implicit that the answer might be No. We believe this question deserves deeper investigation as a future work.

[Question 29]:
 Compute the double integrals over indicated rectangles $\iint_{\text{limits}_R} (2x - 4y^3) \, dA$, $R = [-5, 4] \times [0, 3]$

[Function 0]:

```

python
def double_integral(function, x_limits, y_limits):
    """
    Computes the double integral of a given function over a rectangular region.

    Parameters:
    - function (callable): The function to be integrated. It should take two arguments (x, y).
    - x_limits (tuple): A tuple containing the lower and upper limits of integration for the x-variable.
    - y_limits (tuple): A tuple containing the lower and upper limits of integration for the y-variable.

    Returns:
    - float: The value of the double integral.

    Note:
    - This function uses the scipy library to compute the double integral.
    """
    from scipy.integrate import nquad

    # Define the limits of integration for the x and y variables.
    limits = [x_limits, y_limits]

    # Compute the double integral using the nquad function from scipy.
    result, _ = nquad(function, limits)
    return result
  
```

Let's consider the **[Function 0]**

Retained

Refined

Figure 9: The screenshot of our annotation interface to evaluate functions' generalization.

[Question 0]:
 Square ABCD. Rectangle AEFG. The degree of $\angle AFG = 20$. Please find $\angle AEB$ in terms of degree. Return the numeric value.

[Function 0]:

```

python
def calculate_angle_in_rectangle(angle1, angle2):
    """
    Calculates the angle in a rectangle given two other angles.

    Parameters:
    - angle1 (float): The first angle in degrees.
    - angle2 (float): The second angle in degrees.

    Returns:
    - float: The calculated angle in degrees.
    """
    return angle1 - angle2
  
```

[Solution]:

```

python
# Define the angles
angle_AFB = 45 # in degrees
angle_AFG = 20 # in degrees

# Calculate the angle  $\angle AEB$ 
angle_AEB = calculate_angle_in_rectangle(angle_AFB, angle_AFG)

print(angle_AEB)
  
```

Let's consider to rewrite **[Function 0]**. You can optionally use one of the below alternative functions (if have) for substitution:

Next

Figure 10: The screenshot of our annotation interface to rewrite functions. We provide no alternative functions in this example for convenience of visualization.

Function before rewriting

```
def birge_vieta(p, tol=1e-3, max_iter=100):
    """
    Finds a real root of the polynomial  $x^3 - 11x^2 + 32x - 22$  using the Birge-Vieta method.

    Parameters:
    - p (float): The initial guess for the root.
    - tol (float, optional): The desired tolerance for the root. Default is 1e-3.
    - max_iter (int, optional): The maximum number of iterations. Default is 100.

    Returns:
    - float: The real root of the polynomial found using the Birge-Vieta method.
    """
    for _ in range(max_iter):
        p_new = p - polynomial(p) / polynomial_derivative(p)
        if abs(p_new - p) < tol:
            return p_new
        p = p_new
    raise ValueError("Birge-Vieta method did not converge within the maximum number of iterations.")
```

Rewrite the specific polynomial (and its derivative) to an argument of the function

Function after rewriting

```
def birge_vieta_iteration(polynomial, p, tol=1e-3, max_iter=100):
    """
    Finds a real root of a polynomial using the Birge-Vieta method.

    Parameters:
    - polynomial (sympy expression): The polynomial for which the root is to be found.
    - p (float): The initial guess for the root.
    - tol (float): The desired tolerance for the root.
    - max_iter (int): The maximum number of iterations allowed.

    Returns:
    - float: The real root of the polynomial, if found within the maximum number of iterations.
    - Raises a ValueError if the root is not found within the maximum number of iterations.
    """
    from sympy import lambdify, diff
    import numpy as np

    # Extract the variable from the polynomial
    variables = list(polynomial.free_symbols)
    if not variables:
        raise ValueError("No variables found in the polynomial.")
    if len(variables) > 1:
        raise ValueError("The polynomial contains more than one variable.")
    variable = variables[0]

    # Compute the derivative of the polynomial
    derivative = diff(polynomial, variable)

    # Convert the polynomial and its derivative to functions
    f = lambdify(variable, polynomial, 'numpy')
    f_prime = lambdify(variable, derivative, 'numpy')

    # Iterate using the Birge-Vieta method
    for _ in range(max_iter):
        p_new = p - f(p) / f_prime(p)
        if np.abs(p_new - p) < tol:
            return p_new
        p = p_new
    raise ValueError("Maximum number of iterations reached without convergence.")
```

Function before rewriting

```
def calculate_emptying_time(height, radius, side_length, g=9.81):
    """
    Calculates the time it takes for a cylindrical tank to go from full to empty.

    Parameters:
    - height (float): The height of the cylindrical tank.
    - radius (float): The radius of the cylindrical tank.
    - side_length (float): The length of the side of the square hole in the bottom of the tank.
    - g (float): The acceleration due to gravity.

    Returns:
    - float: The time it takes for the tank to empty.
    """
    from math import pi, sqrt
    # Calculate the area of the tank and the hole
    tank_area = pi * radius**2
    hole_area = side_length**2

    # Use Torricelli's law to calculate the time
    time = (2 * height * tank_area) / (sqrt(2*g*height) * hole_area)
    return time
```

Function after rewriting

```
def calculate_drain_time(volume, area, gravity=9.81):
    """
    Calculates the time it takes for a cylindrical object to drain using Torricelli's Law.

    Parameters:
    - volume (float): The volume of the cylindrical object.
    - area (float): The area of the hole through which the object is draining.
    - gravity (float): The acceleration due to gravity.

    Returns:
    - float: The time it takes for the object to drain.
    """
    from math import sqrt
    return volume / (area * sqrt(2*gravity))
```

1. Abstract the function description by changing "tank" to "object"
2. Decompose the area calculation and Torricelli's law

Function before rewriting

```
def is_log_concave():
    """
    Determines if the cumulative distribution function (CDF) of the standard Gaussian distribution is log-concave.

    Returns:
    - int: 1 if the CDF is log-concave, 0 otherwise.

    Note:
    - The second derivative of the natural logarithm of the CDF of the standard Gaussian distribution is always non-positive.
    - Therefore, the function is log-concave, and we can return 1 without performing any calculations.
    """
    return 1
```

Rewrite the specific function (and its variable) to an argument of the function

Function after rewriting

```
def is_log_concave(f, x):
    """
    Determines if a given function 'f' with respect to variable 'x' is log-concave.

    Parameters:
    - f (sympy expression): The function for which the log-concavity is to be checked.
    - x (sympy symbol): The variable with respect to which log-concavity is to be checked.

    Returns:
    - bool: True if the function is log-concave, False otherwise.
    """
    from sympy import diff, log, simplify, solveset, S
    from sympy.calculus.util import continuous_domain

    # Compute the first derivative of the logarithm of the function
    first_derivative = diff(log(f), x)

    # Compute the second derivative of the logarithm of the function
    second_derivative = diff(first_derivative, x)

    # Simplify the second derivative
    second_derivative_simplified = simplify(second_derivative)

    # Check if the second derivative is nonpositive (<= 0)
    # We check if the second_derivative is nonpositive for all x in the domain of f
    # For a general solution, we attempt to prove the second derivative is always nonpositive
    return solveset(second_derivative_simplified <= 0, domain=S.Reals) == continuous_domain(second_derivative_simplified, x, S.Reals)
```

Figure 11: Three examples of Refined functions (before rewriting) and their rewritten functions (after rewriting). We also briefly describe the modifications for each example (color in red).

G Examples

Problem & Planing

Read the following mathematical question and answer it. Please note that you could (optionally, not required) call the following functions when writing the code:

Question: Suppose a stock has the following information. It is listed on the London stock exchange and operates throughout Europe. The yield on a UK 10 year treasury is 2.8%. The stock in question will earn 8.6% as per historical data. The Beta for the stock is 1.4, i.e., it is 140% volatile to the changes in the general stock market. What is the expected rate of return?

-
- (1) Calculate the expected return based on the beta and the yield on a UK 10 year treasury.
 - (2) Add the stock's historical return to the expected return.

Retrieved Functions

```
def expected_return(rf, beta, rm):
    """
    Computes the expected return using the Capital Asset Pricing Model (CAPM) formula.

    Parameters:
    - rf (float): The risk-free rate.
    - beta (float): The beta of the portfolio.
    - rm (float): The return on the market.

    Returns:
    - float: The expected return.
    """
    return rf + beta * (rm - rf)

def expected_stock_return(true_prob, u, d):
    """
    Calculates the expected return of the stock in a one-period binomial model.

    Parameters:
    - true_prob (float): The true probability of the stock price going up.
    - u (float): One plus the rate of capital gain on the stock if the price goes up.
    - d (float): One plus the rate of capital loss on the stock if the price goes down.

    Returns:
    - float: The expected return of the stock.
    """
    return true_prob * u + (1 - true_prob) * d

...
```

Solution

```
# Given values.
rf = 0.028 # The yield on a UK 10 year treasury
beta = 1.4 # The stock is 140% volatile to the changes in the general stock market
rm = 0.086 # The stock in question will earn 8.6% as per historical data
# Calculate the expected return .
expected_return = expected_return(rf, beta, rm)
# Print the result.
print(expected_return)
```

Figure 12: An example of direct function call.

Problem & Planing

Read the following mathematical question and answer it. Please note that you could (optionally, not required) call the following functions when writing the code:

Question: The linear density in a rod 8 m long is $12 / \sqrt{x+1} \text{ kg} / \text{m}$, where x is measured in meters from one end of the rod. Find the average density of the rod.

- (1) Integrate the linear density function with respect to x from 0 to 8 .
- (2) Divide the result by the length of the rod.

Retrieved Functions

```
def average_value_of_function(f, a, b):
    """
    Calculates the average value of a function `f` on the interval `[a, b]`.
    Parameters: - f (sympy expression): The function for which the average value is to be found.
    - a (float): The lower limit of the interval.
    - b (float): The upper limit of the interval.
    Returns: float: The average value of the function on the interval.
    """
    from sympy import integrate, symbols
    x = symbols('x')
    integral = integrate(f, (x, a, b))
    average_value = integral / (b - a)
    return average_value

def avg_distance(vectors):
    """
    Finds the average distance from the origin that can be reached by adding and subtracting the given
    vectors.
    Parameters: - vectors (list of numpy arrays): The vectors.
    Returns: float: The average distance.
    """
    from itertools import product
    import numpy as np
    total_distance = 0
    count = 0
    for signs in product([-1, 1], repeat=len(vectors)):
        resultant = sum(v * s for v, s in zip(vectors, signs))
        distance = np.linalg.norm(resultant)
        total_distance += distance
        count += 1
    return total_distance / count

...
```

Solution

```
# The linear density is given by 12 / sqrt(x+1) kg/m.
# The average density is the total mass of the rod divided by its length.
# The total mass of the rod is the integral of the linear density times the length of the rod from 0 to
8.
from sympy import symbols, integrate
x = symbols('x')
length = 8
# Define the linear density function.
linear_density = 12 / (x + 1)**0.5
# Calculate the total mass of the rod.
total_mass = integrate(linear_density, (x, 0, length))
# Calculate the average density by dividing the total mass by the length.
average_density = total_mass / length
print(average_density)
```

Figure 13: An example of implicitly using functions as a reference.

H Prompts

H.1 Tool/Function Collection

Listing 5: Prompt used for planning and function collection

```
Given the question and the reference solution, do the following things:

- Think about what math knowledge points are required to solve this problem step by
  step.
- write some python one or more functions to abstract the solution. Please note that
  the functions should be well-documented as much as possible and not too
  specific (for example, do not write the values in this problem within the
  functions. Pass them as the function arguments). We hope your written functions
  could be re-used in anywhere else.
-Instantiate these functions to solve the problem. The last line of your program
  should be a 'print' command to print the final answer

Here are some examples you may refer to:

Question: There are integers  $b, c$  for which both roots of the polynomial  $x^2-x-1$ 
  are also roots of the polynomial  $x^5-bx-c$ . Determine the product  $bc$ .
Answer: Let  $r$  be a root of  $x^2-x-1$ . Then, rearranging, we have  $r^2 = r+1$ .
  Multiplying both sides by  $r$  and substituting gives  $r^3 = r^2+r = (r+1)+r = 2r+1$ . Repeating this process twice
  more, we have  $r^4 = r(2r+1) = 2r^2+r = 2(r+1)+r = 3r+2$  and  $r^5 = r(3r+2) = 3r^2+2r = 3(r+1)+2r = 5r+3$ . Thus, each root of  $x^2-x-1$ 
  is also a root of  $x^5-5x-3$ , which gives  $bc = 5 \cdot 3 = \boxed{15}$ .
Think: To solve this question, we can follow the steps below: (1) Find the roots of
  the polynomial  $x^2-x-1$ . (2) Substitute them into the the polynomial  $x^5-bx-c$ 
  and obtain two equations. (3) Solve the equations.

Functions:
'''function 1
def find_roots_of_polynomial(polynomial, variable):
    """
    Finds the roots of a given polynomial using the sympy library.

    Parameters:
    - polynomial (sympy expression): The polynomial whose roots are to be found.
    - variable (sympy symbol): The variable of the polynomial.

    Returns:
    - list: The roots of the polynomial.
    """
    from sympy import solve
    roots = solve(polynomial, variable)
    return roots
'''

'''function 2
def substitute_roots_into_polynomial(roots, polynomial, variable):
    """
    Substitutes the given roots into the polynomial and returns the resulting
    expressions.

    Parameters:
    - roots (list): The list of roots to be substituted into the polynomial.
    - polynomial (sympy expression): The polynomial into which the roots are to be
      substituted.
    - variable (sympy symbol): The variable of the polynomial.

    Returns:
    - list: The resulting expressions after substituting the roots into the
      polynomial.
    """
    return [polynomial.subs(variable, root) for root in roots]
'''
```



```

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1646
'''function 3
def solve_equations(equations, variables):
    """
    Solves a system of equations for the specified variables using the sympy library.

    Parameters:
    - equations (list of sympy expressions or a single sympy expression):
      The equations to be solved. If solving a single equation, this can be a single
      expression.
    - variables (list of sympy symbols or a single sympy symbol):
      The variables for which the solution is to be found. If solving for a single
      variable, this can be a single symbol.

    Returns:
    - list of dictionaries: Each dictionary represents a solution, with keys being
      the variables and values being their corresponding values.
      If there's only one solution, the list will contain a single dictionary.
    """

    from sympy import solve
    solution = solve(equations, variables, dict=True)
    return solution
'''

Solution:
'''python
# Import required functions and classes from sympy
from sympy import symbols, Eq

# Define the variable and the polynomials
x, b, c = symbols('x b c')
polynomial1 = x**2 - x - 1
polynomial2 = x**5 - b*x - c

# Find the roots of the first polynomial
roots = find_roots_of_polynomial(polynomial1, x)

# Substitute the roots into the second polynomial
resulting_expressions = substitute_roots_into_polynomial(roots, polynomial2, x)

# Set up the equations based on the resulting expressions
equations = [Eq(expr, 0) for expr in resulting_expressions]

# Solve the system of equations for b and c
solutions = solve_equations(equations, (b, c))
# This linear system has only one solution
solution = solutions[0]

# Calculate the product bc
product_bc = solution[b] * solution[c]
print(product_bc)
'''

---

Question: Medians  $\overline{DP}$  and  $\overline{EQ}$  of  $\triangle DEF$  are
perpendicular. If  $DP = 18$  and  $EQ = 24$ , then what is  $DE$ ?
Answer: Point  $G$  is the centroid of  $\triangle DEF$ , so  $DG:GP = EG:GQ = 2:1$ .
Therefore,  $DG = \frac{2}{3}(DP) = 12$  and  $EG = \frac{2}{3}(EQ) = 16$ , so applying the
Pythagorean Theorem to  $\triangle EGD$  gives us  $DE = \sqrt{EG^2 + GD^2} = \sqrt{16^2 + 12^2} = 20$ .

Think: Given two perpendicular medians in a triangle, we need to perform the
following steps: (1) Identify the relationship between the segments of medians
and the centroid. (2) Use the ratios provided to determine the lengths of the
individual segments from the centroid to the vertices. (3) Use the Pythagorean
theorem to determine the length of the side connecting the two vertices from
which the medians originate.

Functions:
'''function 1

```

```

1647 def median_segments_length(median_length, ratio):
1648     """
1649     Computes the lengths of the segments of a median split by the centroid.
1650
1651     Parameters:
1652     - median_length (float): Total length of the median.
1653     - ratio (tuple): Ratio in which the centroid splits the median. Default is (2,1)
1654       for standard triangles.
1655
1656     Returns:
1657     - tuple: Lengths of the two segments.
1658
1659     Formula:
1660     - segment_1 = ratio[0]/sum(ratio) * median_length
1661     - segment_2 = ratio[1]/sum(ratio) * median_length
1662     """
1663     segment_1 = ratio[0] / sum(ratio) * median_length
1664     segment_2 = ratio[1] / sum(ratio) * median_length
1665     return segment_1, segment_2
1666
1667
1668
1669 def pythagorean_theorem(a, b):
1670     """
1671     Computes the hypotenuse of a right triangle given two legs.
1672
1673     Parameters:
1674     - a, b (float): Lengths of the two legs.
1675
1676     Returns:
1677     - float: Length of the hypotenuse.
1678
1679     Formula:
1680     - c = sqrt(a^2 + b^2)
1681     """
1682     from sympy import sqrt
1683     return sqrt(a**2 + b**2)
1684
1685
1686 Solution:
1687 ```python
1688 # Given values
1689 DP = 18
1690 EQ = 24
1691
1692 # Point $G$ is the centroid.
1693 ratio = (2,1)
1694 # Determine the lengths of the segments split by the centroid
1695 DG, GP = median_segments_length(DP, ratio)
1696 EG, GQ = median_segments_length(EQ, ratio)
1697
1698 # Use Pythagoras theorem to determine DE
1699 DE = pythagorean_theorem(EG, DG)
1700 print(DE)
1701 ```

```

1703 H.2 Self-rectification

Listing 6: Prompt used for self-rectification

```

1704 {
1705     "role": "system",
1706     "content": "Suppose you are writing Python programs to solve mathematical
1707       questions. Your original program, however, can not run normally for some
1708       reasons. Given the error message returned from the interpreter, please debug
1709       your program carefully and generate the new program. Your generated
1710       correction MUST FOLLOW the following format:\n```function 1\n[the first
1711       created function]\n```\n...\n```function N\n[the N-th created function]\n```\n

```

```

    ``python\n[solution]\n``.\nDO NOT only quote your output as ``python\n[
solution]\n``"
},
{
"role": "user",
"content": "Original Program:\n``function 1\ndef solve_quadratic(a, b, c):\n
from sympy import symbols, Eq, solve\n x = symbols('x')\n quadratic = Eq(a *
x**2 + b * x + c, 0)\n solutions = solve(quadratic, x)\n return solutions\n
``\n\n``python\ndef find_d_values():\n a, b, c, d = symbols('a b c d')\n eq1
= Eq(6 * a * d, a + d)\n eq2 = Eq((6 * d - 1) * (1 - a), a + d)\n eq3 = Eq(a,
4 * d - 1)\n solution = solve([eq1, eq2, eq3], (a, b, c, d), dict=True)\n
d_values = [sol[d] for sol in solution]\n return d_values\n d_values =
find_d_values()\n print(d_values)\n``\n\nError Message:\nFile <string>:15\n
nFile <string>:9, in find_d_values()\n\nNameError: name 'Eq' is not defined"
},
{
"role": "assistant",
"content": "Analysis: The error is occurring because the Eq function from the
sympy module is not recognized in the find_d_values function. This is
happening because the ``from sympy import symbols, Eq, solve`` line is only
inside the ``solve_quadratic`` function, so Eq and other imported functions
and classes are only available within the scope of that function. To fix this,
you should claim import statement within the ``find_d_values`` function as
well.\n\nNew Program:\n``function 1\ndef solve_quadratic(a, b, c):\n
from sympy import symbols, Eq, solve\n x = symbols('x')\n quadratic = Eq(a * x**2
+ b * x + c, 0)\n solutions = solve(quadratic, x)\n return solutions\n``\n\n
``python\ndef find_d_values():\n from sympy import symbols, Eq, solve\n a, b,
c, d = symbols('a b c d')\n eq1 = Eq(6 * a * d, a + d)\n eq2 = Eq((6 * d -
1) * (1 - a), a + d)\n eq3 = Eq(a, 4 * d - 1)\n solution = solve([eq1, eq2,
eq3], (a, b, c, d), dict=True)\n d_values = [sol[d] for sol in solution]\n
return d_values\n d_values = find_d_values()\n print(d_values)\n``"
},
{
"role": "user",
"content": "finished"
},
{
"role": "user",
"content": "Original Program:\n``function 1\ndef matrix_square(matrix):\n
from sympy import Matrix\n if not isinstance(matrix, Matrix):\n matrix = Matrix(
matrix)\n return matrix * matrix\n``\n\n``function 2\ndef solve_equations(
equations, variables): \n from sympy import solve \n solution = solve(
equations, variables, dict=True) \n return solution\n``\n\n``function 3\
ndef count_solutions(solutions):\n return len(solutions)\n``\n\n``python\
nfrom sympy import symbols, Eq \na, d = symbols('a d') \nmatrix = [[a, 3],
[-8, d]] \nsquared_matrix = matrix_square(matrix) \nidentity_matrix = [[1, 0],
[0, 1]] \nequations = [Eq(squared_matrix[i][j], identity_matrix[i][j]) for i
in range(2) for j in range(2)] \nsolution = solve_equations(equations, [a, d
]) \nans = count_solutions(solution)\n print(ans)\n``\n\nError Message:\nFile
<string>:17\n\nFile <string>:17, in <listcomp>(.0)\n\nTypeError: 'Add'
object is not subscriptable"
},
{
"role": "assistant",
"content": "Analysis: The error message is occurring because when you are
creating the list of equations with the list comprehension, squared_matrix[i
][j] is not working as expected. The squared_matrix is a SymPy Matrix object,
and you should use the .row and .col methods.\n\nNew Program:\n``function 1\
ndef matrix_square(matrix):\n from sympy import Matrix\n if not isinstance(
matrix, Matrix):\n matrix = Matrix(matrix)\n return matrix * matrix\n``\n\n
``function 2\ndef solve_equations(equations, variables): \n from sympy
import solve \n solution = solve(equations, variables, dict=True) \n return
solution\n``\n\n``function 3\ndef count_solutions(solutions):\n return len(
solutions)\n``\n\n``python\nfrom sympy import symbols, Eq \na, d = symbols('
a d') \nmatrix = [[a, 3], [-8, d]] \nsquared_matrix = matrix_square(matrix) \
nidentity_matrix = [[1, 0], [0, 1]] \nequations = [Eq(squared_matrix.row(i)[j
], identity_matrix[i][j]) for i in range(2) for j in range(2)] \nsolution =
solve_equations(equations, [a, d]) \nans = count_solutions(solution)\n print(
ans)\n``"
},

```

```

1784 {
1785     "role": "user",
1786     "content": "finished"
1787 },
1788 {
1789     "role": "user",
1790     "content": "Original Program:\n```function 1\ndef sum_to_product_cos(alpha, beta)
1791     :\n return (cmath.cos(alpha - beta) + cmath.cos(alpha + beta)) / 2\n```\n\n```
1792     function 2\ndef simplify_expression(expression): \n from sympy import
1793     simplify \n return simplify(expression) \n```\n\n```python\nfrom sympy import
1794     symbols, cos\n\nx = symbols('x')\nexpr = cos(x) + cos(3*x) + cos(7*x) + cos
1795     (9*x)\n\n# Apply sum-to-product formula\nexpr1 = 2 * sum_to_product_cos(5*x,
1796     4*x)\nexpr2 = 2 * sum_to_product_cos(5*x, 2*x)\n\n# Simplify the expression\n
1797     nsimplified_expr = simplify_expression(expr1 + expr2)\n\n# Extract the values
1798     of a, b, c, and d and sum them up\na, b, c, d = 4, 1, 3, 5\nans = a + b + c
1799     + d\nprint(ans)\n```\n\nError Message:\nFile <string>:12\n\nFile <string>:2,
1800     in sum_to_product_cos(alpha, beta)\n\nNameError: name 'cmath' is not defined"
1801 },
1802 {
1803     "role": "assistant",
1804     "content": "Analysis: The error message is occurring because the cmath module is
1805     being used in the sum_to_product_cos function but it has not been imported.
1806     You can fix this by importing the cmath module in this function. New Program
1807     :\n```function 1\ndef sum_to_product_cos(alpha, beta):\n import cmath\n
1808     return (cmath.cos(alpha - beta) + cmath.cos(alpha + beta)) / 2\n```\n\n```
1809     function 2\ndef simplify_expression(expression): \n from sympy import
1810     simplify \n return simplify(expression)\n```\n\n```python\nfrom sympy import
1811     symbols, cos\n\nx = symbols('x')\nexpr = cos(x) + cos(3*x) + cos(7*x) + cos
1812     (9*x)\n\n# Apply sum-to-product formula\nexpr1 = 2 * sum_to_product_cos(5*x,
1813     4*x)\nexpr2 = 2 * sum_to_product_cos(5*x, 2*x)\n\n# Simplify the expression\n
1814     nsimplified_expr = simplify_expression(expr1 + expr2)\n\n# Extract the values
1815     of a, b, c, and d and sum them up\na, b, c, d = 4, 1, 3, 5\nans = a + b + c
1816     + d\nprint(ans)\n```\n"
1817 },
1818 {
1819     "role": "user",
1820     "content": "Error message:\nTraceback (most recent call last):\n File, line 9, in
1821     <module>\n exec(\n File '<string>', line 13, in <module>\n File '<string>',
1822     line 3, in sum_to_product_cos\n File, line 356, in __complex__\n return
1823     complex(float(re), float(im))\n File, line 351, in __float__\n raise
1824     TypeError('Cannot convert expression to float')\nTypeError: Cannot convert
1825     expression to float\n"
1826 },
1827 {
1828     "role": "assistant",
1829     "content": "Analysis: The error occurs because you are trying to use cmath.cos
1830     function (which expects float or complex numbers as arguments) with SymPy
1831     symbolic expressions (5x and 4x, 5x and 2x are symbolic expressions). To fix
1832     this, you should use SymPy's cos function instead of cmath.cos function to
1833     work with symbolic expressions.\n\nNew Program:\ndef sum_to_product_cos(alpha,
1834     beta):\n from sympy import cos\n return (cos(alpha - beta) + cos(alpha +
1835     beta)) / 2\ndef simplify_expression(expression): \n from sympy import
1836     simplify \n return simplify(expression) \nfrom sympy import symbols, cos\n\nx
1837     = symbols('x')\nexpr = cos(x) + cos(3*x) + cos(7*x) + cos(9*x)\n\n# Apply
1838     sum-to-product formula\nexpr1 = 2 * sum_to_product_cos(5*x, 4*x)\nexpr2 = 2 *
1839     sum_to_product_cos(5*x, 2*x)\n\n# Simplify the expression\nnsimplified_expr =
1840     simplify_expression(expr1 + expr2)\n\n# Extract the values of a, b, c, and d
1841     and sum them up\na, b, c, d = 4, 1, 3, 5\nans = a + b + c + d\nprint(ans)"
1842 },
1843 {
1844     "role": "user",
1845     "content": "finished"
1846 },
1847 {
1848     "role": "user",
1849     "content": "Original Program:\n```function 1\ndef tan_double_angle(tan_theta):\n
1850     return 2 * tan_theta / (1 - tan_theta**2)\n```\n\n```function 2\ndef
1851     tan_triple_angle(tan_theta):\n return (3 * tan_theta - tan_theta**3) / (1 - 3
1852     * tan_theta**2)\n```\n\n```function 3\ndef solve_polynomial(polynomial, x):\n
1853     from sympy import solve\n return solve(polynomial, x)\n```\n\n```python\nfrom

```

```

    sympy import symbols\ntan_theta = symbols('tan_theta')\ntan_2_theta =          1854
tan_double_angle(tan_theta)\ntan_3_theta = tan_triple_angle(tan_theta)\          1855
nequation = tan_theta + tan_2_theta + tan_3_theta\nsimplified_equation =          1856
simplify_expression(equation)\ntan_theta_solutions = solve_polynomial(          1857
simplified_equation, tan_theta)\n\n# Find the solution in the given range (0          1858
< tan_theta < 1)\ntan_theta_value = [solution for solution in          1859
tan_theta_solutions if 0 < solution < 1][0]\nprint(tan_theta_value)\n```\n          1860
nErrorMessage:\nFile <string>:13\n\nNameError: name 'simplify_expression' is          1861
not defined"          1862
},          1863
{          1864
    "role": "assistant",          1865
    "content": "Analysis: The error message is occurring because there is no function          1866
named simplify_expression defined in your script. To fix this, you can          1867
define such a function that uses SymPy's simplify function to simplify          1868
expressions.\n\nNew Program:\n```\nfunction 1\ndef simplify_expression(          1869
expression): \n from sympy import simplify \n return simplify(expression)\n          1870
```\n\n```\nfunction 2\ndef tan_double_angle(tan_theta):\n return 2 * tan_theta          1871
/ (1 - tan_theta**2)\n```\n\n```\nfunction 3\ndef tan_triple_angle(tan_theta):\n 1872
return (3 * tan_theta - tan_theta**3) / (1 - 3 * tan_theta**2)\n```\n\n```\n 1873
function 4\ndef solve_polynomial(polynomial, x):\n from sympy import solve\n 1874
return solve(polynomial, x)\n```\n\n```\npython\nfrom sympy import symbols\ 1875
ntan_theta = symbols('tan_theta')\ntan_2_theta = tan_double_angle(tan_theta)\ 1876
ntan_3_theta = tan_triple_angle(tan_theta)\nequation = tan_theta + 1877
tan_2_theta + tan_3_theta\nsimplified_equation = simplify_expression(equation 1878
)\ntan_theta_solutions = solve_polynomial(simplified_equation, tan_theta)\n\n 1879
Find the solution in the given range (0 < tan_theta < 1)\ntan_theta_value = 1880
[solution for solution in tan_theta_solutions if 0 < solution < 1][0]\nprint 1881
(tan_theta_value)\n```\n 1882
}, 1883
{ 1884
 "role": "user", 1885
 "content": "finished" 1886
} 1887
} 1888

```

### H.3 Function-augmented Solutions

Listing 7: Prompt used for the generation of function-augmented solutions (cross-retrieval strategy)

```

You will encounter a mathematical problem and are required to write a piece of 1890
Python code to solve this problem. 1891

Now we have a suite of wrapped functions. Take note: 1892
- The newly provided wrapped functions have NOT been verified. They may be 1893
irrelevant or potentially flawed. 1894
- It's essential that the solution doesn't overly depend on wrapped functions. 1895
You're welcome to utilize one or more functions from the new set in your solution 1896
but only after you've determined: 1897
(1) Their accuracy. 1898
(2) Their inclusion significantly streamlines the problem-solving approach. 1899

Additionally take note that 1900
(1) The last line of your written code shall be a 'print' command to print the 1901
final answer. 1902
(2) The wrapped functions should not be duplicated within your code. Instead, 1903
call them directly if needed. 1904
(3) Should you need to create custom functions, do so without adding 1905
documentation comments for the sake of brevity. 1906
(4) Write simple but clear annotations interleaving your code solution. 1907

"""\ 1908
Retrieved functions: 1909
[List of called function names from the new set] 1910

```python          1911
[Your Written Python Code.]          1912
"""\          1913

```

```

1921 For example:
1922 ---
1923 Question: What is the 100th digit to the right of the decimal point in the decimal
1924 representation of  $\frac{13}{90}$ ?
1925
1926 New provided functions:
1927 ```New Function 0
1928 def decimal_representation(numerator, denominator, max_digits=1000):
1929     """
1930     Computes the decimal representation of a fraction.
1931
1932     Parameters:
1933     - numerator (int): The numerator of the fraction.
1934     - denominator (int): The denominator of the fraction.
1935     - max_digits (int): The maximum number of decimal digits to compute.
1936
1937     Returns:
1938     - str: The decimal representation of the fraction as a string.
1939     """
1940
1941     result = ""
1942     remainder = numerator % denominator
1943     for _ in range(max_digits):
1944         remainder *= 10
1945         result += str(remainder // denominator)
1946         remainder %= denominator
1947         if remainder == 0:
1948             break
1949     return result
1950 ...
1951
1952 ```New Function 1
1953 def decimal_to_scientific(decimal_number):
1954     from sympy import log, floor
1955     exponent = -floor(log(decimal_number, 10))
1956     coefficient = decimal_number * 10**(-exponent)
1957     return coefficient, exponent
1958 ...
1959
1960 ```New Function 2
1961 def repeating_decimal_representation(numerator, denominator):
1962     """
1963     Computes the repeating decimal representation of a fraction.
1964
1965     Parameters:
1966     - numerator (int): The numerator of the fraction.
1967     - denominator (int): The denominator of the fraction.
1968
1969     Returns:
1970     - str: The repeating decimal representation of the fraction as a string.
1971     """
1972
1973     # Initialize the result string and a dictionary to store remainders.
1974     result = ""
1975     remainders = {}
1976
1977     # Perform long division to find the decimal representation.
1978     while numerator != 0:
1979         # If the remainder has been seen before, we found the repeating block.
1980         if numerator in remainders:
1981             start = remainders[numerator]
1982             return result[:start] + "(" + result[start:] + ")"
1983         # Otherwise, store the remainder and continue the division.
1984         remainders[numerator] = len(result)
1985         numerator *= 10
1986         result += str(numerator // denominator)
1987         numerator %= denominator
1988
1989     return result
1990 ...

```

```

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2059
2060
```New Function 3
def nth_digit_of_decimal_representation(numerator, denominator, n):
 """
 Computes the nth digit after the decimal point of the decimal representation of a
 fraction.

 Parameters:
 - numerator (int): The numerator of the fraction.
 - denominator (int): The denominator of the fraction.
 - n (int): The position of the digit after the decimal point.

 Returns:
 - int: The nth digit after the decimal point of the decimal representation of the
 fraction.
 """

 # Get the repeating decimal representation of the fraction.
 decimal_representation = repeating_decimal_representation(numerator, denominator)

 # Remove the parentheses from the repeating block.
 decimal_representation = decimal_representation.replace("(", "").replace(")", "")

 # Calculate the nth digit using the repeating block.
 return int(decimal_representation[(n - 1) % len(decimal_representation)])
...

Retrieved functions:
[decimal_representation, nth_digit_of_decimal_representation]

```python
# Use the nth_digit_of_decimal_representation function to find the 100th digit
numerator = 13
denominator = 90
n = 100

# Call the function and print the result
result = nth_digit_of_decimal_representation(numerator, denominator, n)
print(result)
```

Question: The square root of x^2 is greater than 3 and less than 4. How many integer
values of x^2 satisfy this condition?

New provided functions:
```New Function 0
def solve_square_root_equation(a, b, c):
    """
    Solves a square root equation of the form  $\sqrt{ax - b} = c$ .

    Parameters:
    - a (float): Coefficient of x inside the square root.
    - b (float): Constant term inside the square root.
    - c (float): Constant term on the right side of the equation.

    Returns:
    - float: The value of x that satisfies the equation.

    Formula:
    -  $x = (c^2 + b) / a$ 
    """
    return (c**2 + b) / a
...

```New Function 1
def find_integer_square_less_than_double():
 """
 Finds the only integer whose square is less than its double.

```

```

2061
2062 Returns:
2063 - int: The integer that satisfies the condition.
2064
2065 Method:
2066 - Iterate through integers starting from 1, and check if the square of the
2067 integer is less than its double.
2068 - If the condition is satisfied, return the integer.
2069 - If the condition is not satisfied for any integer up to a certain limit, return
2070 None.
2071 """
2072 limit = 100
2073 for x in range(1, limit):
2074 if x**2 < 2*x:
2075 return x
2076 return None
2077 ...
2078
2079 ```New Function 2
2080 def solve_equation():
2081 """
2082 Solves the equation $(x-2)^{(25-x^2)} = 1$ for integer solutions.
2083
2084 Returns:
2085 - list: A list of integer solutions for x.
2086 """
2087 solutions = []
2088
2089 # Case 1: Exponent is 0 ($25 - x^2 = 0$)
2090 x1 = 5
2091 x2 = -5
2092 solutions.extend([x1, x2])
2093
2094 # Case 2: Base is 1 ($x - 2 = 1$)
2095 x3 = 3
2096 solutions.append(x3)
2097
2098 # Case 3: Base is -1 and exponent is even ($x - 2 = -1$ and $25 - x^2 = 2n$ for some
2099 integer n)
2100 x4 = 1
2101 solutions.append(x4)
2102
2103 return solutions
2104 ...
2105
2106 ```New Function 3
2107 def count_integers_in_range(lower_bound, upper_bound, exclude_zero=True):
2108 """
2109 Counts the number of integers within a given range.
2110
2111 Parameters:
2112 - lower_bound (int): The lower bound of the range.
2113 - upper_bound (int): The upper bound of the range.
2114 - exclude_zero (bool): Whether to exclude 0 from the count. Default is True.
2115
2116 Returns:
2117 - int: The number of integers within the range.
2118 """
2119 count = upper_bound - lower_bound + 1
2120 if exclude_zero and lower_bound <= 0 and upper_bound >= 0:
2121 count -= 1
2122 return count
2123 ...
2124
2125 Retrieved functions:
2126 []
2127
2128 ```python
2129 # The lower and upper bounds of x for which $\sqrt{x} > 3$ and $\sqrt{x} < 4$
2130 lower_bound = 9

```



```

upper_bound = 16
Counting the number of integers between 9 (exclusive) and 16 (exclusive)
num_integers = len([x for x in range(lower_bound + 1, upper_bound)])

Printing the result
print(num_integers)

```

## H.4 Evaluation with Toolsets

Listing 8: Prompt used for evaluation (setting with toolsets)

Read the following questions and answer them. For each question, you are required to write a Python program to solve it. Please note that we provide you several functions for each question. You could (optionally, not required) call the functions to help you to solve the question if necessary. Note that the last line of your program should be a 'print' command to print the final answer

-----  
Question:

What is the 100th digit to the right of the decimal point in the decimal representation of  $\frac{13}{90}$ ?

Functions:

```

def repeating_decimal_representation(numerator, denominator):
 """
 Computes the repeating decimal representation of a fraction.

 Parameters:
 - numerator (int): The numerator of the fraction.
 - denominator (int): The denominator of the fraction.

 Returns:
 - str: The repeating decimal representation of the fraction as a string.
 """

 # Initialize the result string and a dictionary to store remainders.
 result = ""
 remainders = {}

 # Perform long division to find the decimal representation.
 while numerator != 0:
 # If the remainder has been seen before, we found the repeating block.
 if numerator in remainders:
 start = remainders[numerator]
 return result[:start] + "(" + result[start:] + ")"
 # Otherwise, store the remainder and continue the division.
 remainders[numerator] = len(result)
 numerator *= 10
 result += str(numerator // denominator)
 numerator %= denominator

 return result

def nth_digit_of_decimal_representation(numerator, denominator, n):
 """
 Computes the nth digit after the decimal point of the decimal representation of a fraction.

 Parameters:
 - numerator (int): The numerator of the fraction.
 - denominator (int): The denominator of the fraction.
 - n (int): The position of the digit after the decimal point.

 Returns:
 """

```

```

2198 - int: The nth digit after the decimal point of the decimal representation of the
2199 fraction.
2200 """
2201
2202 # Get the repeating decimal representation of the fraction.
2203 decimal_representation = repeating_decimal_representation(numerator, denominator)
2204
2205 # Remove the parentheses from the repeating block.
2206 decimal_representation = decimal_representation.replace("(", "").replace(")", "")
2207
2208 # Calculate the nth digit using the repeating block.
2209 return int(decimal_representation[(n - 1) % len(decimal_representation)])
2210
2211
2212 def decimal_representation(numerator, denominator, max_digits=1000):
2213 """
2214 Computes the decimal representation of a fraction.
2215
2216 Parameters:
2217 - numerator (int): The numerator of the fraction.
2218 - denominator (int): The denominator of the fraction.
2219 - max_digits (int): The maximum number of decimal digits to compute.
2220
2221 Returns:
2222 - str: The decimal representation of the fraction as a string.
2223 """
2224
2225 result = ""
2226 remainder = numerator % denominator
2227 for _ in range(max_digits):
2228 remainder *= 10
2229 result += str(remainder // denominator)
2230 remainder %= denominator
2231 if remainder == 0:
2232 break
2233 return result
2234
2235
2236 Solution:
2237 # find the 100th digit.
2238 numerator = 13
2239 denominator = 90
2240 n = 100
2241
2242 # Call the function and print the result.
2243 result = nth_digit_of_decimal_representation(numerator, denominator, n)
2244 print(result)
2245
2246 -----
2247
2248 Question:
2249 The square root of x^2 is greater than 3 and less than 4. How many integer values of
2250 x^2 satisfy this condition?
2251
2252 Functions:
2253 def count_integers_in_range(lower_bound, upper_bound, exclude_zero=True):
2254 """
2255 Counts the number of integers within a given range.
2256
2257 Parameters:
2258 - lower_bound (int): The lower bound of the range.
2259 - upper_bound (int): The upper bound of the range.
2260 - exclude_zero (bool): Whether to exclude 0 from the count. Default is True.
2261
2262 Returns:
2263 - int: The number of integers within the range.
2264 """
2265 count = upper_bound - lower_bound + 1
2266 if exclude_zero and lower_bound <= 0 and upper_bound >= 0:
2267 count -= 1

```

```

return count
2268
2269
2270
def find_integer_square_less_than_double():
2271
2272
 """
2273
 Finds the only integer whose square is less than its double.
2274
 Returns:
2275
 - int: The integer that satisfies the condition.
2276
2277
 Method:
2278
 - Iterate through integers starting from 1, and check if the square of the
2279
 integer is less than its double.
2280
 - If the condition is satisfied, return the integer.
2281
 - If the condition is not satisfied for any integer up to a certain limit, return
2282
 None.
2283
 """
2284
 limit = 100
2285
 for x in range(1, limit):
2286
 if x**2 < 2*x:
2287
 return x
2288
 return None
2289
2290
2291
def solve_square_root_equation(a, b, c):
2292
2293
 """
2294
 Solves a square root equation of the form sqrt(ax - b) = c.
2295
2296
 Parameters:
2297
 - a (float): Coefficient of x inside the square root.
2298
 - b (float): Constant term inside the square root.
2299
 - c (float): Constant term on the right side of the equation.
2300
2301
 Returns:
2302
 - float: The value of x that satisfies the equation.
2303
2304
 Formula:
2305
 - $x = (c^2 + b) / a$
2306
 """
2307
 return (c**2 + b) / a
2308
2309
2310
Solution:
2311
We need to find the integer values of x for which sqrt(x) > 3 and sqrt(x) < 4. To
2312
 this end, we can count the number of integers in the range (9, 16) directly.
2313
result = 0
2314
for x in range(10, 16):
2315
 if 9 < x < 16:
2316
 result += 1
2317
print(result)
2318

```

## H.5 Evaluation without Toolsets 2319

### Listing 9: Prompt used for evaluation (setting without toolsets)

```

Read the following questions and answer them. For each question, you are required to
2320
 write a Python program to solve it.
2321
2322
Please note that we provide you several functions for each question. You could (
2323
 optionally, not required) call the functions to help you to solve the question
2324
 if necessary.
2325
Note that the last line of your program should be a 'print' command to print the
2326
 final answer
2327

2328
Question:
2329
What is the 100th digit to the right of the decimal point in the decimal
2330
 representation of $\frac{13}{90}$?
2331
2332
Solution:
2333
2334

```

```

2335 from decimal import Decimal, getcontext
2336
2337 # Set the precision to 101 (100 digits after decimal + 1 digit before decimal)
2338 getcontext().prec = 101
2339
2340 # Calculate the decimal representation of 13/90
2341 dec = Decimal(13) / Decimal(90)
2342
2343 # Convert the decimal to a string
2344 dec_str = str(dec)
2345
2346 # Get the 100th digit to the right of the decimal point
2347 digit_100th = dec_str[101]
2348
2349 print(digit_100th)
2350
2351 -----
2352 Question:
2353 The square root of x is greater than 3 and less than 4. How many integer values of
2354 x satisfy this condition?
2355
2356 Solution:
2357 # We need to find the integer values of x for which $\sqrt{x} > 3$ and $\sqrt{x} < 4$. To
2358 this end, we can count the number of integers in the range (9, 16) directly.
2359 result = 0
2360 for x in range(10, 16):
2361 if 9 < x < 16:
2362 result += 1
2363 print(result)

```

---