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ABSTRACT

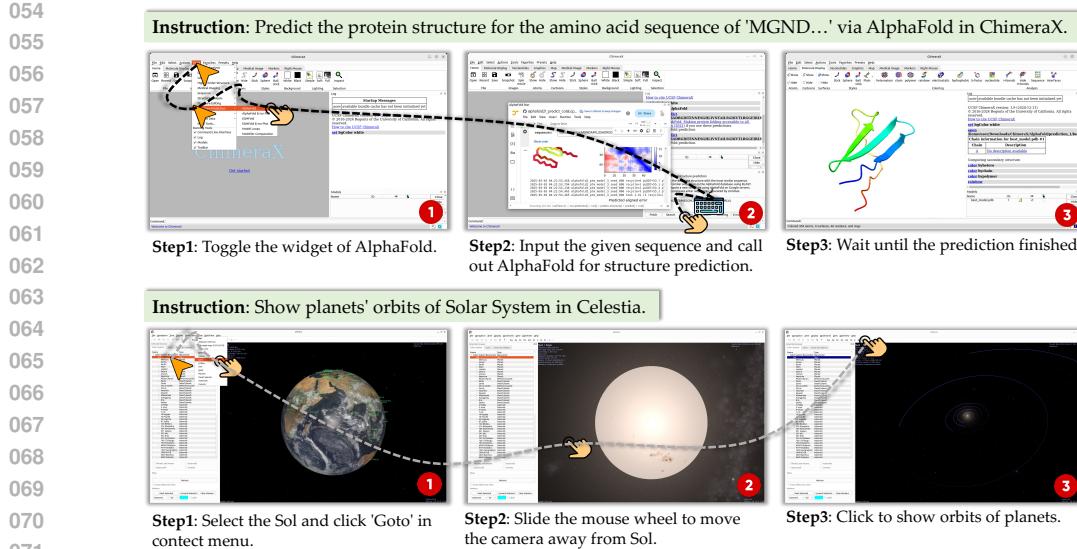
Large Language Models (LLMs) have extended their impact beyond Natural Language Processing, substantially fostering the development of interdisciplinary research. Recently, various LLM-based agents have been developed to assist scientific discovery progress across multiple aspects and domains. Among these, computer-using agents, capable of interacting with operating systems as humans do, are paving the way to automated scientific problem-solving and addressing routines in researchers’ workflows. Recognizing the transformative potential of these agents, we introduce SCIENCEBOARD, which encompasses two complementary contributions: (i) a realistic, multi-domain environment featuring dynamic and visually rich scientific workflows with integrated professional software, where agents can autonomously interact via different interfaces to accelerate complex research tasks and experiments; and (ii) a challenging benchmark of 169 high-quality, rigorously validated real-world tasks curated by humans, spanning scientific-discovery workflows in domains such as biochemistry, astronomy, and geoinformatics. Extensive evaluations of agents with state-of-the-art backbones (*e.g.*, GPT-4o, Claude 3.7, UI-TARS) show that, despite some promising results, they still fall short of reliably assisting scientists in complex workflows, achieving only a 15% overall success rate. In-depth analysis further provides valuable insights for addressing current agent limitations and more effective design principles, paving the way to build more capable agents for scientific discovery. Our code, benchmark, and leaderboard are available at <https://anonymous.4open.science/r/ScienceBoard/>.

1 INTRODUCTION

In the pursuit of scientific advances, researchers combine ingenuity and expertise to perform novel research grounded in experimental explorations. In the modern era, scientific discovery is increasingly driven by specialized software and tools that empower scientists to engage deeply with the experimental world (Hacking, 1983). Tools like simulation engines (Hollingsworth & Dror, 2018), data analysis software (The MathWorks Inc., 2022), and visualization platforms (Goddard et al., 2018) are essential for formulating hypotheses, validating results, and advancing scientific understanding.

However, as scientific software grows more sophisticated and workflows become more demanding, the learning curve and operational burden on human researchers intensify (Sänger et al., 2024). These challenges motivate the vision of autonomous agents to play a central role in automating research pipelines and assisting human researchers as “AI co-scientists” (Luo et al., 2025; Schmidgall et al., 2025; Gottweis et al., 2025). For example, while a human scientist may take weeks to master a protein analysis tool (Meng et al., 2023) and spend hours making sufficient observations, an autonomous agent could perform the same tasks within minutes. By enabling fully autonomous workflows—from tool usage to making novel discoveries (Lu et al., 2024a)—such agents promise to accelerate science and empower researchers with unprecedented capabilities.

Recently emerging computer-using agents (Wu et al., 2024; OpenAI, 2025), capable of operating digital devices in a human-like manner, present a promising approach toward achieving these visions. These agents can interact with operating systems through Command-Line Interfaces (CLI; Sun et al., 2024a; Wang et al., 2024d) or perform mouse and keyboard actions via Graphical User



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108 computer tasks as humans do, leading to the proliferation of computer-using agents (OpenAI, 2025).
 109 One line of research utilizes Command Line Interface (CLI), where agents generate executable scripts
 110 (*e.g.*, Python or Shell scripts) to interact with systems programmatically (Wang et al., 2024b). In this
 111 process, agents perform code synthesis (Sun et al., 2024a) or invoke APIs (Wu et al., 2024; Zhang
 112 et al., 2024). Another line of research focuses on Graphical User Interface (GUI) agents (Cheng et al.,
 113 2024; Wu et al., 2025b; Lin et al., 2024) that interact with digital devices through human-like mouse
 114 and keyboard actions (Niu et al., 2024; Zheng et al., 2024; Gou et al., 2025). These agents transform
 115 user instructions into executable actions within the operating system (*e.g.*, clicking an icon or scrolling
 116 through a page). Powered by VLMs, GUI agents have been applied to automate desktop (Xie et al.,
 117 2024) and mobile (Rawles et al., 2025) tasks, as well as specialized engineering workflows (Cao et al.,
 118 2024), showing promising paths toward digital automation. This work innovatively initiates the use
 119 of computer agents in scientific workflows, taking a step closer to autonomous research assistants.
 120

121 **AI for Scientific Discovery.** The rapid advancement of LLMs has reshaped the landscape of
 122 scientific discovery (Microsoft, 2023), boosting multiple stages of the research cycle (Luo et al.,
 123 2025). With the rise of LLM/VLM-based agents, there is a growing demand for these game-
 124 changers with college-level knowledge (Wang et al., 2024a) to transcend traditional tasks like
 125 question answering (Lu et al., 2022; Krishnareddy et al., 2023; Lu et al., 2024b). Recent efforts have
 126 been directed towards harnessing such power to assist with diverse components of the research cycle,
 127 including idea and hypothesis generation (Si et al., 2024; Liu et al., 2024b), data analysis (Chen
 128 et al., 2025; Gu et al., 2024; Majumder et al., 2024), scientific programming (Tian et al., 2024;
 129 Novikov et al., 2025), paper writing (Wang et al., 2024c), and peer-reviewing (Yu et al., 2024).
 130 Meanwhile, incorporating domain knowledge or even constructing foundation models (Microsoft,
 131 2025) can endow these agents with the capability to solve domain-specific problems, such as theorem
 132 proving (Song et al., 2025), chemical reasoning (Ouyang et al., 2024; Tang et al., 2025) and biological
 133 discovery (Wang et al., 2025; Zhao et al., 2025; Wang et al., 2025; Frey et al., 2025). With the vision
 134 of constructing autonomous research assistants (Schmidgall et al., 2025), our work represents the
 135 first to support agents in executing end-to-end scientific exploration workflows, thereby laying a
 136 cornerstone for advancing AI-powered scientific discovery.
 137

3 SCIENCEBOARD ENVIRONMENT

138 In this part, we introduce SCIENCEBOARD environment, which encompasses real-world science
 139 software that could be manipulated through GUI and CLI interfaces. The interface is developed
 140 based on an Ubuntu virtual machine (VM), serving as the underlying infrastructure. The dynamic and
 141 visually intensive environments distinguish SCIENCEBOARD from all previous works that evaluate
 142 the scientific capabilities of models or agents.
 143

3.1 PRELIMINARIES AND TASK DEFINITION

144 A computer-using agent receives task instructions, selects actions to manipulate software, and receives
 145 feedback reflecting changes in the environment (tabletop). This interaction is modeled as a Partially
 146 Observable Markov Decision Process (POMDP), defined by the tuple $\langle g, \mathcal{S}, \mathcal{A}, \mathcal{O}, \mathcal{T} \rangle$, where g is the
 147 goal, \mathcal{S} is the state space, \mathcal{A} is the action space, \mathcal{O} is the observation space (including environment
 148 feedback), and $\mathcal{T} : \mathcal{S} \times \mathcal{A} \rightarrow \mathcal{S}$ is the state transition function. Given a policy π , the agent
 149 predicts actions at each time step t based on the goal g and memory $m_t = o_j, a_j, o_{j+1}, a_{j+1}, \dots, o_t$
 150 ($0 \leq j < t$), which records the sequence of past actions and observations. The trajectory $\tau =$
 151 $[s_0, a_0, s_1, a_1, \dots, s_t]$ is determined by the policy and environment dynamics:
 152

$$p_\pi(\tau) = p(s_0) \prod_{t=0}^T \pi(a_t | g, s_t, m_t) \mathcal{T}(s_{t+1} | s_t, a_t) \quad (1)$$

153 **Observation and Memory.** We evaluate computer agents using three types of observation spaces:
 154 text-only, visual-only, and combined text-visual observations. For text-based observations, we
 155 use accessibility trees (a11ytree¹) to generate structured textual representations of screenshots.
 156 For visual observations, we capture high-resolution screenshots directly. The specific observation
 157 combinations used in our experiments are detailed in Section 5.1, with further information in
 158
 159
 160
 161

¹a11ytree: Accessibility (a11y) trees are hierarchical structures representing UI elements on the screen.

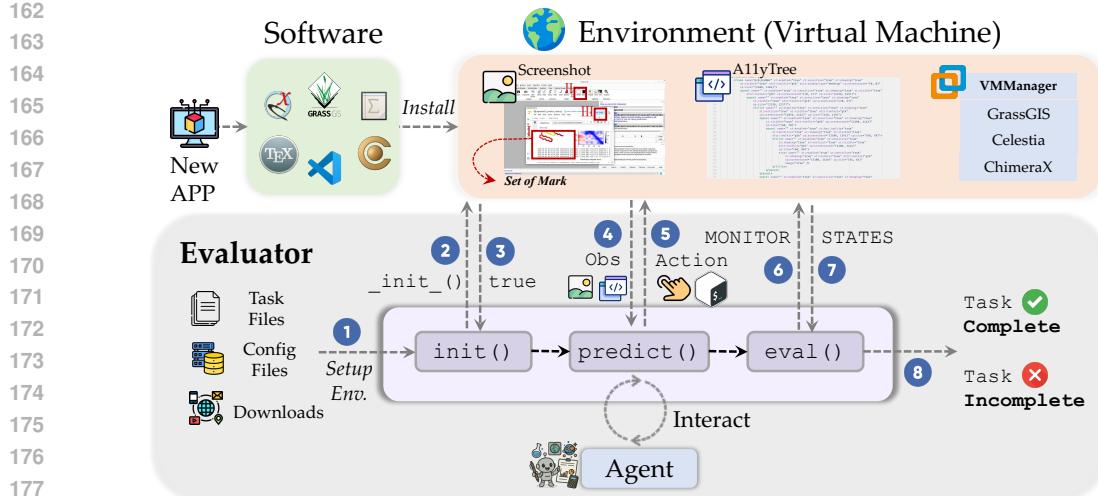


Figure 2: Overview of the SCIENCEBOARD infrastructure. The scalable environment is built upon a VM pre-installed with scientific discovery software. It supports both CLI and GUI interfaces to enable autonomous agent interaction. For each task designed to evaluate the agent’s capability as a research assistant, an initialization script, configs, and related files are provided. Agents perceive the environment through visual or textual modalities, and are expected to plan and act accordingly. After the interaction, an evaluation function determines completion based on the VM internal states.

Appendix B.5. Our POMDP agent requires memory to retain historical information. Following previous work (Yao et al., 2023; Ma et al., 2024), we construct this memory by concatenating the agent’s most recent observations.

Goal and Unified Action Space. Each task is specified by a natural language (NL) instruction, such as `Display atoms in sphere style`, describing the user’s intended goal. The policy model decomposes a complex goal instruction into a sequence of actions. We specially design a unified action space \mathcal{A} in SCIENCEBOARD, integrating diverse interaction modalities crucial for scientific tasks. For GUI actions, agents can perform the full range of human-computer interactions, including mouse movements, clicks, keystrokes, and other typical input behaviors as in prior work (Xie et al., 2024; Zhou et al., 2024) (e.g., `CLICK [991, 019]`). For CLI actions, agents can interact at two levels: (a) invoking system-level commands within the Ubuntu terminal, and (b) utilizing application-specific CLI or scripting mechanisms. Moreover, \mathcal{A} comprises an `answer` action, enabling agents to provide specific answers for QA tasks, and a `call_api` action, allowing agents to leverage predefined external APIs to broaden their capabilities. A comprehensive list of supported action types is available in Appendix B.4.

LLM/VLM-based Policy Model. An LLM / VLM model acts as the policy model to drive the agent’s behavior. The policy model receives the current observation and generates the next action accordingly. For pure-text observation, we adopt LLMs as the policy. Otherwise, we leverage VLMs.

3.2 SCIENTIFIC DISCOVERY EVALUATION FRAMEWORK

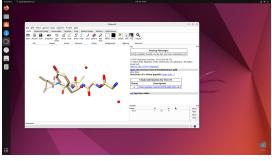
Unlike prior work that primarily focuses on static QA, coding, or single-step tasks, we aim to provide agents with a realistic and visually grounded environment to support autonomous exploration, which in turn introduces greater challenges for planning and action. In SCIENCEBOARD environment, as shown in Figure 2, we (1) simulate scenarios where scientific software is used to solve domain-specific problems, (2) enable agents to interact with the environment through diverse observations, and (3) ensure that agent behaviors can be rigorously evaluated.

Scientific Software Installation and Adaptation. For each domain, we select an open-source application that supports both visual and textual observations as the agent’s playground. To enable access to the internal state of each application within the VM, we adapt the software accordingly. Given the complexity and limited completeness of scientific applications, we inject a lightweight server that launches alongside the application’s main UI process to expose internal states via HTTP requests. This server is capable of querying the application’s runtime internal states, which serve as

the basis for downstream evaluation. For applications that do not natively support remote control via RESTful APIs, we modify and recompile their source code to ensure that both UI elements and internal states can be accessed. In addition, the server supports partial state control of the software, allowing us to initialize with specific configurations to simulate contextualized task environments. More about the software selected and further implementation details are provided in Appendix B.3.

Agent Interactions with the Environment. The LLM/VLM agent interacts with the environment as described in Section 3.1, receiving observations and executing actions accordingly. Scientific software processes these actions and returns updated states. The agent operates autonomously, continuing this loop until it outputs a signal (DONE or FAIL) or reaches the predefined attempt limit.

Table 1: Typical evaluation cases of SCIENCEBOARD include exact matching, range-based assessment, and numerical tasks with tolerance. We have tailored appropriate evaluation methods for each task. Additional evaluation strategies are detailed in Appendix D.4.

Initial State	Instruction	Evaluation Script (Simplified)
	Select all water molecules and draw their centroids with radius of 1Å in ChimeraX.	<pre>{ "type": "info", "key": "sell", "value": ["atom id #!1/A:201@O idatm_type O3", "..."], }, { "type": "states", "find": "lambda k,v:k.endswith('.name')", "key": "lambda k:'..._atoms_drawing'", "value": "[[13.0012 1.7766 21.3672 1.]]" } }</pre>
	Display and ONLY display the layer of 'boundary_region' in Grass GIS.	<pre>{ "type": "info", "key": "lambda dump:len(dump['layers'])", "value": 1 }, { "type": "info", "key": "lambda dump:dump['layers'][0]['name']", "value": "boundary_region@PERMANENT" }</pre>
	Set the Julian date to 2400000 in Celestia.	<pre>{ "type": "info", "key": "simTime", "value": 2400000, "pred": "lambda left, right:abs(left-right) < 1", }</pre>

Evaluation Pipeline. Given the complexity of scientific tasks, conventional answer-matching metrics and even execution-based evaluations (Xie et al., 2024; Zhou et al., 2024), often lack the granularity required to assess workflows accurately. For instance, as shown in Table 1, the rotation of a protein does not affect the correctness of visualization, whereas computational tasks in astronomy are usually influenced by the current clock state. Therefore, we propose a fine-grained evaluation based on both the correctness of key I/O during the workflow and the final state of the VM.

To handle the diverse criteria for determining task correctness (*e.g.*, exact matching, range-based assessment, numerical tolerance, file comparison), we design a set of evaluation templates. For each specific task, the relevant template is then instantiated with the appropriate parameters and expected gold standard values. This ensures both consistent validation and scalability for future extension. More evaluation details are in Appendix B.2.

4 SCIENCEBOARD BENCHMARK

In this section, we present the covered domains, the annotation pipeline, and statistics of the benchmark constructed based on the SCIENCEBOARD environment.

4.1 DOMAIN AND TASK COVERAGE

As a pioneering benchmark for scientific exploration, SCIENCEBOARD spans six domains selected for their relevance to key stages of the scientific workflow, such as simulation, modeling, prediction, and knowledge (Microsoft, 2023). In selecting software for each domain, we consider not only its representativeness, but also practical criteria for evaluation: open-source availability, allytree compatibility, and no requirement for user authentication.

270 (1) **Biochemistry.** We employ UCSF ChimeraX (Goddard et al., 2018; Meng et al., 2023), a
 271 molecular analysis tool that supports structural modeling (e.g., AlphaFold (Jumper et al., 2021)).
 272 The tasks assess the agent’s ability to manipulate biomolecular structures, as well as to reason
 273 over spatial conformations and biochem annotations.

274 (2) **Algebra.** KAlgebra is employed to evaluate the agent’s potential in symbolic mathematics.
 275 Tasks involve executing algebraic expressions, interpreting plots, and manipulating symbolic
 276 functions. These scenarios require the agent to exhibit strong mathematical symbolic reasoning
 277 and visual grounding capability.

278 (3) **Theorem Proving.** We use Lean 4 (Moura & Ullrich, 2021) as a proof assistant to assess
 279 agents’ abilities in formal logic and deductive reasoning. The ATP tasks in this category
 280 emphasize syntactic precision and logical coherence, evaluating the agent’s capability to generate
 281 semantically valid formal proofs.

282 (4) **Geographic Information System.** GrassGIS, a computational engine for raster, vector, and
 283 geospatial processing, is included to examine the agent’s skills in understanding terrain, hydrology,
 284 and handling spatio-temporal data, with support for functions such as ecosystem modeling.

285 (5) **Astronomy.** We integrate Celestia, a planetarium software simulating real-world astronomi-
 286 cal scenarios. Agents must demonstrate temporal-spatial awareness and knowledge of the cosmos
 287 and celestial objects by tracking planetary systems, simulating orbital events, and querying object
 288 metadata across time and space.

289 (6) **Scientific Documentation.** To simulate research documentation workflows, we adapt and
 290 incorporate TeXstudio to assess the agent’s technical writing capabilities. In standalone tasks,
 291 agents are expected to compose well-structured abstracts, generate plots, and produce formal
 292 reports based on provided instructions. In cross-application scenarios, TeXstudio is coupled
 293 with the aforementioned software to evaluate whether agents can extract meaningful insights
 294 from experiments and synthesize them into coherent narratives.

295 These domains enable evaluating a science agent’s capabilities across multiple dimensions, including
 296 visual / textual reasoning, math, coding, tool use, spatial understanding, domain-specific knowledge,
 297 and more. Additionally, to explore the potential for end-to-end scientific automation, documentation
 298 tasks are integrated with other domains to support cross-application workflows—such as automatically
 299 generating an experimental report based on completed upstream tasks. More details about the software
 300 platforms used to instantiate and convey the tasks in SCIENCEBOARD are provided in Appendix B.3.

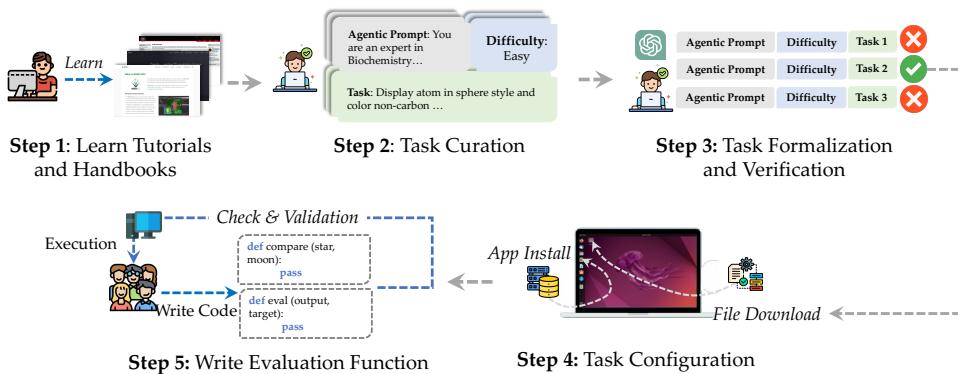


Figure 3: The annotation pipeline of the tasks in SCIENCEBOARD benchmark.

4.2 TASK ANNOTATION PIPELINE

To effectively construct tasks that are appropriately challenging, diverse, and aligned with the features of scientific software, we leverage a pipeline that spans from training annotators with tutorials and handbooks to conducting execution-based validation, as shown in Figure 3.

(1) **Tutorial Learning.** Five annotators initially collect and learn from tutorials and handbooks related to the software. After that, each annotator studies and explores a software’s basic unit operations, e.g., plotting the Bernoulli lemniscate in KAlgebra. Details are in Appendix D.1.

(2) **Task Curation.** Each annotator selects a scientific software, installs it within SCIENCEBOARD, and begins drafting task instructions based on its functionalities. Task types include but are not

324 limited to: configuration, simulation, QA, and domain-specific expertise. Each task is tentatively
 325 assigned a difficulty. Thereafter, agentic prompts aligned with the drafted tasks will be curated.
 326 (3) **Formalization and Selection.** Different annotators exhibit varying linguistic habits, we employ
 327 ChatGPT to standardize the task format. Annotators then conduct a cross-check, excluding those
 328 lacking diversity, poor executability, or non-unique answers, to finalize the set of tasks for use.
 329 (4) **Configuration Function Writing.** The purpose of this step is to initialize the software and pro-
 330 vide specific contexts, *e.g.*, supplying a map for GIS tasks or a protein sequence for biochemistry
 331 tasks. Annotators will write a set of functions for each software to modify the VM status, *i.e.*,
 332 the internal state of the software, along with general configuration functions (*e.g.*, downloading
 333 required files). Tasks commence only after all initialization have been successfully executed.
 334 (5) **Evaluation Function Writing and Validation.** Evaluation functions are developed to assess
 335 task outcomes rigorously. As described in Section 3.2, evaluations are state-based, with functions
 336 derived from a base evaluator template. Annotators retrieve the task state from the VM and assess
 337 it based on criteria such as I/O matching and predefined ranges. The function returns either “task
 338 complete” or “task fail.” Cross-validation is performed for consistency, with each task executed
 339 by two randomly selected annotators on separate VMs. The results are analyzed to ensure the
 340 evaluator’s correctness, even under intentional attempts by annotators to deceive the system.
 341

4.3 TASK STATISTICS

342 The task statistics of SCIENCEBOARD benchmark are presented in Table 2. Specifically, it comprises
 343 169 unique tasks across 6 domains, with task difficulty categorized into three levels. We curate a
 344 balanced number of tasks that are representative enough while keeping the evaluation cost manageable.
 345 During annotation, we define multiple task types to evaluate agents’ ability to perform diverse
 346 operation flows and leverage domain-specific knowledge.
 347

348 Table 2: Statistics of SCIENCEBOARD.
 349

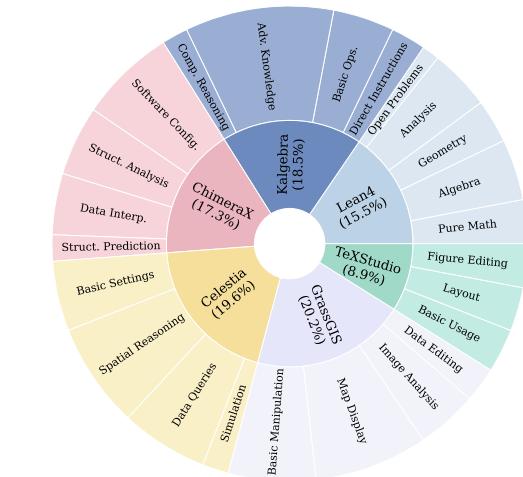
Task Type	Statistics
Total Tasks	169 (100%)
- GUI	38 (22.5%)
- CLI	33 (19.5%)
- GUI + CLI	98 (58.0%)
Difficulty	
- Easy	91 (53.8%)
- Medium	48 (28.4%)
- Hard	28 (16.6%)
- Open Problems	2 (1.2%)
Instructions	
Avg. Length of Task Instructions	20.0
Avg. Length of Agentic Prompt	374.9
Execution	
Avg. Steps	9.0
Avg. Time Consumption	124(s)

366 The distribution of task types is shown in Figure 4. Beyond the innovation of a realistic environment,
 367 SCIENCEBOARD benchmark also improves upon prior work in terms of task design and content
 368 diversity. More details about task diversity, stability analysis, and comparison with representative
 369 scientific benchmarks are provided in Appendix D.
 370

5 EXPERIMENTS

5.1 EXPERIMENTAL SETTINGS

374 **Backbones.** We employ three types of backbones for agents. These include **proprietary models**: GPT-4o (Hurst et al., 2024), Claude-3.7-Sonnet (Anthropic AI, 2024),
 375 Gemini-2.0-Flash (Team, 2024), and o3-mini (OpenAI, 2025); **open-source models**: Qwen2.5-VL-72B-Instruct (Bai et al., 2025), InternVL3-78B (Chen et al., 2024), QvQ-72B-
 376 Preview (Qwen Team, 2024), and GPT-oss-120B (Open AI, 2025); and **GUI action models**: OS-
 377



378 Atlas-Pro-7B (Wu et al., 2025b), UGround-V1-7B (Gou et al., 2025), UI-TARS-72B-DPO / UI-
 379 TARS-1.5-7B (Qin et al., 2025), and GUI-Actor-7B (Wu et al., 2025a). More details in Appendix E.1.
 380

381 **Observation Space.** We follow established observation settings (Xie et al., 2024; Zhou et al., 2024):
 382 (1) full desktop screenshots; (2) `allytree`, a structured text-only representation; (3) Screenshots +
 383 `allytree`; and (4) Set-of-Marks (Yang et al., 2023), which partitions images into marked regions
 384 to aid grounding. Further details are in Appendix B.5.

385 5.2 RESULTS

387 We compare the performance of computer-use agents powered by different LLMs and VLMs on
 388 SCIENCEBOARD, as presented in Table 3. We summarize our key empirical findings as follows:
 389

390 Table 3: Success rates on SCIENCEBOARD. We present the performance of each agent back-
 391 bone across different scientific domains under various observation settings. Proprietary Models ,
 392 Open-Source VLMs / LLMs , and GUI Action Model are distinguished by color.

393 Observations	394 Model	395 Success Rate (↑)						
		396 Algebra	397 Biochem	398 GIS	399 ATP	400 Astron	401 Doc	402 Overall
396 Screenshot	GPT-4o	3.23%	0.00%	0.00%	0.00%	0.00%	6.25%	1.58%
	Claude-3.7-Sonnet	9.67%	37.93%	2.94%	0.00%	6.06%	6.25%	10.48%
	Gemini-2.0-Flash	6.45%	3.45%	2.94%	0.00%	0.00%	6.06%	3.15%
	Qwen2.5-VL-72B	22.58%	27.59%	5.88%	0.00%	9.09%	12.50%	12.94%
	InternVL3-78B	6.45%	3.45%	0.00%	0.00%	0.00%	6.25%	2.69%
	UI-TARS-1.5-7B	12.90%	13.79%	0.00%	0.00%	6.06%	0.00%	2.69%
402 allytree	GPT-4o	12.90%	20.69%	2.94%	0.00%	6.06%	0.00%	7.10%
	Claude-3.7-Sonnet	19.35%	34.48%	2.94%	3.85%	12.12%	0.00%	12.12%
	Gemini-2.0-Flash	9.68%	17.24%	0.00%	0.00%	0.00%	0.00%	4.49%
	o3-mini	16.13%	20.69%	2.94%	3.85%	15.15%	6.25%	10.84%
	Qwen2.5-VL-72B	9.68%	10.34%	2.94%	0.00%	3.03%	0.00%	4.33%
	InternVL3-78B	3.23%	3.45%	0.00%	0.00%	0.00%	0.00%	1.11%
	GPT-oss-120B	19.35%	13.79%	0.00%	0.00%	9.09%	0.00%	7.04%
409 Screenshot + allytree	GPT-4o	22.58%	37.93%	2.94%	7.69%	3.03%	12.50%	14.45%
	Claude-3.7-Sonnet	12.90%	41.37%	8.82%	3.85%	9.09%	18.75%	15.79%
	Gemini-2.0-Flash	16.13%	24.14%	2.94%	0.00%	18.18%	12.50%	12.32%
	Qwen2.5-VL-72B	16.13%	20.69%	2.94%	0.00%	18.18%	12.50%	11.74%
	InternVL3-78B	6.45%	3.45%	0.00%	0.00%	3.03%	6.25%	3.20%
	Human Performance	74.19%	68.97%	55.88%	42.31%	51.52%	68.75%	60.27%

422 **Performance Hierarchy.** Existing agents remain far from being capable of effectively assisting
 423 human scientists in completing real-world scientific exploration tasks. Even SOTA models, such
 424 as GPT-4o and Claude, achieve an average success rate of only 15%. Across various settings,
 425 open-source counterparts can partially match proprietary models. However, they still exhibit markedly
 426 lower overall performance, with an average success rate of less than 12% and approaching nearly 0%
 427 in some task categories. The gap between agent and human performance underscores the limitations
 428 of the status quo and necessitates further research.

429 **Domain-Specific Performance Insights.** Across domains, we observe clear performance imbal-
 430 ances: models perform moderately well on Algebra and Biochemistry but degrade notably on GIS
 431 and Astronomy. We attribute this to: (1) Interfaces: Algebra and Biochemistry tasks often support
 both CLI and GUI execution, whereas GIS and Astronomy rely mainly on GUI interactions. Agents

432 generally handle CLI commands more reliably than fine-grained GUI grounding, which demands
 433 precise visual localization. (2) Task emphasis: Geographical and astronomical tasks involve dense
 434 visual elements (e.g., maps, star charts), making it difficult for agents to identify and reason over
 435 relevant information. This also indicates the limited 3D spatial reasoning ability of current VLMs.

436 **Impact of Different Observations.** Different observation modalities have a significant impact.
 437 Overall, `a11ytree + screenshots` setting yields the best performance. In other settings, Qwen2.5-VL
 438 performs exceptionally well under screenshot setting, which we attribute to its advanced GUI ability.
 439 Under `a11ytree`, the attribute information of elements allows LLMs to complete certain tasks by
 440 relying solely on textual observations. Meanwhile, we observe that the SoM sometimes introduces
 441 negative effects. It is likely that although SoM provides bounding boxes to ease grounding, scientific
 442 software often contains massive elements on screen (e.g., dense celestial objects and complex cosmic
 443 backgrounds), which introduces substantial noise and increases the difficulty of visual reasoning.

444 6 ANALYSIS

445 To further investigate the factors influencing agents’ capabilities, we conduct additional analysis to
 446 understand the underlying causes and the behavioral differences among heterogeneous models.

447 **Disentangled Planning and Action.** Observations from failure cases indicate that some models,
 448 such as GPT-4○, can effectively plan tasks but lack sufficient grounding capabilities. Therefore, we
 449 explore separating planning and action. Following existing practices (Wu et al., 2025b), we configure
 450 GPT-4○ as the planner and utilize various VLMs and GUI action models as the grounding models.

451 Table 4: Success rates of different VLM agent combinations under the planner + grounding model
 452 setting on SCIENCEBOARD. The observation setting used in this experiment is screenshot. Colors
 453 denote Proprietary Models, Open-Source VLMs and GUI Action Models.

455 Planner	456 Grounding Model	457 Success Rate (↑)				
		458 Algebra	459 Biochem	460 GIS	461 Astron	462 Overall
463 GPT-4○	464 OS-Atlas-Pro-7B	465 6.25%	466 10.34%	467 0.00%	468 3.03%	469 4.92%
	470 UGround-V1-7B	471 0.00%	472 3.45%	473 0.00%	474 3.03%	475 1.62%
	476 Qwen2.5-VL-72B	477 12.50%	478 34.48%	479 11.76%	480 9.09%	481 16.96%
	482 UI-TARS-72B	483 3.23%	484 10.34%	485 5.88%	486 6.06%	487 6.38%
	488 GUI-Actor-7B	489 21.88%	490 44.83%	491 2.94%	492 12.12%	493 20.44%
494 GPT-4○		495 3.23%	496 0.00%	497 0.00%	498 0.00%	499 0.81%

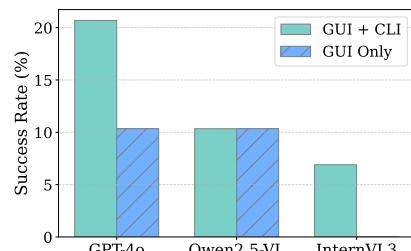
500 The results in Table 4 show that modular approaches yield significant improvements and are promising
 501 for tackling complex and visually demanding tasks in scientific software workflows.

502 **GUI vs. Hybrid.** Some tasks support both GUI and CLI as interchangeable interfaces. For
 503 example, ChimeraX offers nearly full functional coverage through both modes for biochemistry tasks.
 504 To test how computer-using agents handle such hybrid software, we disable ChimeraX’s CLI, enforcing GUI-
 505 only execution (`a11ytree + screenshot`). As shown in Figure 5, GPT-4○ and InternVL3 suffer clear drops
 506 in performance, whereas Qwen2.5-VL remains largely unaffected, indicating better adaptation to GUI execution.

507 These results suggest that future agents should be more
 508 adaptable and equipped with stronger GUI capabilities
 509 to remain robust across hybrid and vision-only settings.
 510 Extended analyses are provided in Appendix F.

511 7 CONCLUSION

512 We propose SCIENCEBOARD, a first-of-its-kind realistic environment designed to empower au-
 513 tonomous agents in scientific exploration with rigorous validation. Building upon our infrastructure,
 514 we curate a highly challenging benchmark of diverse scientific tasks meticulously crafted by human
 515 experts. Through extensive experiments and analysis, we found that even state-of-the-art computer-
 516 using agents perform significantly below human-level proficiency. Although the realization of
 517 autonomous agents for scientific discovery remains a distant goal, this work offers actionable insights
 518 for future development, and we believe it constitutes advancing AI-powered scientific discovery.



519 Figure 5: GUI + CLI v.s. GUI Only.

486 REPRODUCIBILITY STATEMENT
487488 We provide an anonymous downloadable source code at [this link](#). The deployment process of
489 SCIENCEBOARD is detailed in Appendix C, while the experimental settings for running evaluations
490 on SCIENCEBOARD are described in Section 5.1.
491492 ETHICS STATEMENT
493494 Computer-using agents operating in live OS environments could potentially affect the normal func-
495 tioning of the system. This is non-negligible in scientific workflows, where a poorly controlled
496 agent could potentially misconfigure experiments, corrupt sensitive research data, or even lead to
497 irreversible data loss. However, considering that all settings in this work are conducted within isolated
498 virtual environments, we do not view this as a concern.
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843 LARGE LANGUAGE MODEL USAGE

844
 845 In this submission, we employed LLMs to aid and polish writing, including grammar and typo
 846 checking, as well as for identifying related works.

847 LIMITATIONS AND BROADER IMPACTS

848
 849 As a pioneering effort marking the early stages of integrating computer-using agents into scientific
 850 workflows, it is important to acknowledge certain limitations. While our current evaluation, based on
 851 both VM states and key I/O correctness, provides robust validation, its reliance on a binary success
 852 flag may not fully capture process correctness or partial task completion (e.g., an agent succeeding
 853 in most steps but failing at a final one). Introducing a “partial credit” could offer more granular
 854 evaluation, but accurately defining and implementing such a system for open-ended, OS-level tasks
 855 within diverse scientific software presents significant challenges due to vast state / action spaces. One
 856 potential direction for improvement is to introduce VLMs to serve as judges capable of assigning
 857 partial credit and providing richer feedback. We leave this as future work.

859 A DISCUSSION AND FUTURE DIRECTIONS

860
 861 SCIENCEBOARD represents a significant advance in using autonomous agents for scientific workflows.
 862 Our findings suggest several key directions for future research:

864 **Harmonized Domain Knowledge and Agentic Capability.** Our evaluations suggest that one
 865 contributing factor to current agents’ limitations in scientific exploration is their insufficient domain
 866 knowledge. For instance, the GUI action models we evaluated, while effective at automation, lack
 867 the specialized understanding required for complex scientific tasks. Therefore, future advancements
 868 may focus on enhancing domain-specific abilities, such as enhancing scientific comprehension (Li
 869 et al., 2024), learning from highly relevant resources such as manuals and tutorials, and enabling
 870 on-demand knowledge retrieval (Lála et al., 2024). A key challenge will be to effectively harmonize
 871 this specialized knowledge with general agentic capabilities (Xu et al., 2024a).

872 **Collaborative and Specialized Agents as a Solution.** Analysis in Table 4 indicates that even a
 873 basic modular approach of separating planning and action to different agents can yield significant
 874 performance improvements in complex scientific software workflows. This points toward developing
 875 sophisticated multi-agent systems composed of specialized, heterogeneous agents (Jia et al., 2024a;
 876 Ghafarollahi & Buehler, 2024; Agashe et al., 2025). For example, responsibilities could be disentangled
 877 by assigning planning to agents capable of deep reasoning (Li et al., 2025), action execution to
 878 specialized GUI action models (Wu et al., 2025b; Xu et al., 2024b), and domain-specific capability
 879 to models in particular disciplines (Microsoft, 2023; 2025). These agents could be plug-and-play,
 880 allowing flexible application across broader aspects of the scientific lifecycle, such as data analysis
 881 (Chen et al., 2025), scientific plotting (Jia et al., 2024b), and paper revision (Yu et al., 2024).
 882 While promising, it also demands more sophisticated multi-agent designs to manage and coordinate
 883 the intricate and multifaceted nature of scientific tasks.

884 **Extending Digital Agents to Physical Laboratory.** Current AI-assisted scientific workflows are
 885 primarily at the digital level, focusing on tasks such as data analysis, simulation, and software control.
 886 A natural and impactful next step is to extend the capabilities of such autonomous agents, as fostered
 887 and benchmarked in SCIENCEBOARD, into physical laboratory environments. This transition involves
 888 interfacing agents with robotic systems (Burger et al., 2020; Angelopoulos et al., 2024), applying
 889 principles of embodied AI to perceive and interact with the physical world. Agents would manipulate
 890 laboratory instruments and samples, carry out experimental protocols, and monitor physical processes
 891 in real time, thereby fostering a “lab-in-the-loop” (Frey et al., 2025) future where experimentation
 892 and AI-driven methods are mutually reinforcing.

893 B DETAILS OF SCIENCEBOARD ENVIRONMENT

894 B.1 ENVIRONMENT SETUP

895 Virtual machines can operate their own kernel and system, enabling compatibility with a wide variety
 896 of operating systems. For experiments covered in this paper, we utilize a Linux environment (Ubuntu
 897 22.04.1 LTS with kernel 6.8.0-57-generic) running on x64 personal computers.

901 B.2 EVALUATION CRITERIA

902 As stated in Section 3.2, we employ a fine-grained evaluation methodology based on:

- 903 • The final state of the VM (Determinant)
- 904 • I/O states and intermediate steps (Non-Determinant)

905 While the final state of the VM often provides a determinant measure of overall task completion,
 906 the diverse nature of I/O and intermediate steps necessitates a varied set of criteria. The following
 907 outlines the primary principles applied for I/O correctness:

911 • Exact Match:

- 912 – Strict equality: The output or relevant state must be exactly identical to the gold standard (e.g.,
 913 for specific textual outputs or numerical values).
- 914 – Set equality of lines: For multi-line textual outputs, the content of all lines must match the gold
 915 standard, but their order may not be strictly enforced.
- 916 – Question-answering: The agent’s provided answer to a question is compared against a correct
 917 answer or set of acceptable answers.

918 • **Predicate Satisfaction:** Verifying if specific information and generated outputs satisfy predefined
 919 logical conditions or predicates. This includes:
 920

- Value Existence: A required value, file, or UI element is present as expected.
- Value Non-Existence: A specified value, file, or UI element is correctly absent.
- Range Check: A numerical output or parameter falls within a predefined acceptable range (often with a specified tolerance).

925 • **Correct Task Failure (FAIL):** The agent correctly identifies a task as infeasible or terminates
 926 appropriately when unable to complete the objective, outputting a designated FAIL signal.

927 • **Domain-Specific Success Markers:** For certain domains, unique success criteria are employed:
 928

- Lean Tasks: Successful compilation of the generated Lean proof code is considered a primary
 929 indicator.

931 **B.3 SELECTION AND MODIFICATION OF SCIENTIFIC SOFTWARE**
 932

933 To ensure both technical feasibility and representative task diversity, we selected software tools based
 934 on the following criteria:

935

1. **Accessibility.** The software must be open-source or freely available, allowing transparent integration
 936 and reproducibility of experiments.
2. **GUI Compatibility.** The software must expose a usable accessibility tree (a11y tree) to support
 937 fine-grained GUI grounding and interaction.
3. **Domain Representativeness.** The software should be representative of key scientific and technical
 938 domains, enabling meaningful assessment of multimodal agent capabilities across different types
 939 of tasks.

943 Based on these principles, we selected the following software for each target domain:
 944

945

- **Lean.** A functional programming language and interactive theorem prover grounded in dependent
 946 type theory (specifically Martin-Löf Type Theory). Lean enables formal verification of mathematical
 947 theorems and software correctness through rigorous type checking and logical inference,
 948 supporting robust development of maintainable and accurate code.
- **ChimeraX.** A next-generation molecular visualization software developed by UCSF, designed for
 949 detailed interactive exploration, visualization, and analysis of protein and biomolecular structures.
 950 ChimeraX enhances performance and user experience compared to its predecessor, UCSF Chimera,
 951 offering improved graphics rendering, extensibility via plugins, and streamlined workflows for
 952 structural biology research.
- **KAlgebra.** An educational calculator and graphical plotting application within the KDE Education
 953 Project. It supports a wide range of numerical, logical, symbolic, and analytical computations,
 954 enabling users to visualize mathematical functions interactively in both two-dimensional (2D) and
 955 three-dimensional (3D) environments, thus effectively bridging computational mathematics and
 956 educational usability.
- **Celestia.** A cross-platform, interactive real-time 3D astronomical simulation software that allows
 957 users to explore the universe through detailed, dynamic visualizations. Celestia is highly extensible
 958 via scripting, empowering educational and professional users to model and visualize celestial
 959 phenomena and space missions with precision and customization.
- **GrassGIS.** An advanced Geographic Information System (GIS) supporting both raster and vector
 960 geospatial data, along with powerful analytical capabilities for spatial modeling, hydrological
 961 analysis, and environmental simulations. GrassGIS includes a comprehensive Python API for
 962 automation and custom analysis, enabling complex geospatial and temporal analyses tailored to
 963 diverse research and application scenarios.
- **TeXstudio.** An integrated L^AT_EX editor that provides a writing environment tailored specifically
 964 for creating and managing complex technical and scientific documents. TeXstudio enhances
 965 productivity through features such as syntax highlighting, real-time document preview, automatic
 966 reference checking, and intuitive assistance tools, greatly simplifying the process of technical
 967 writing and document preparation.

972 B.4 DETAILS OF ACTION SPACE
973

974 The action space employed in SCIENCEBOARD is shown in Table 5. We combine standard interaction
975 primitives (such as GUI operations) with the flexibility of system-level and application-specific
976 Command-Line Interfaces (CLIs), and has been further expanded with several augmented actions
977 tailored for scientific workflows.

978
979 Table 5: Action space of SCIENCEBOARD environment.
980

Action	Description
moveTo(x, y)	Moves the mouse to the target coordinate.
moveRel(x, y)	Moves the mouse by an offset from current position.
dragTo(x, y)	Drags the mouse to the target coordinate.
dragRel(x, y)	Drags the mouse by an offset from current position.
click(x, y)	Clicks at the target coordinate.
rightClick(x, y)	Performs a right click at the target coordinate.
middleClick(x, y)	Performs a middle click at the target coordinate.
doubleClick(x, y)	Performs double clicks at the target coordinate.
tripleClick(x, y)	Performs triple clicks at the target coordinate.
mouseDown(x, y, button)	Presses a mouse button down.
mouseUp(x, y, button)	Releases a mouse button up.
DONE	Agent decides the task is finished.
FAIL	Agent decides the task is infeasible.
WAIT [n]	Agent decides it should wait, 'n' defaults to 5(s).
ANS [s]	Agent decides it should submit an answer, 's' denotes the answer.
API [name, args]	Invokes a registered API call with name and arguments.
CODE	Run a generated code script (for in-app / system-level tasks, or custom functions).

996
997 B.5 DETAILS OF OBSERVATION SPACE
998

1000 We primarily adhere to well-established settings (Xie et al., 2024; Zhou et al., 2024) for observation
1001 space, encompassing: (1) Screenshots, which consist of a full desktop screenshot as observed by
1002 human users; (2) `allytree`, a structured text-only representation without visual information,
1003 applicable for agents that take pure text input; (3) Screenshots + `allytree`, a hybrid approach
1004 that combines and complements both textual and visual modalities; and (4) Set-of-Marks (Yang
1005 et al., 2023), a visual prompting method aimed at enhancing the visual grounding capabilities by
1006 partitioning an image into marked regions. Details are as follows:

1007 **Screenshot.** We capture a screenshot of the entire computer screen. For screen resolution, we
1008 set a default value of 1920×1080, and it also offers a 16:9 aspect ratio. Following OSWorld (Xie
1009 et al., 2024), our environment also supports modifying the resolution of virtual machines to avoid
1010 potential memorization of absolute pixel values and to assist studies on topics like generalization
1011 across different resolutions.

1012 **A11ytree.** An `allytree` refers to an intricate structure generated by the browser or OS accessibility
1013 APIs that renders a representative model of the content, providing a means of interaction for
1014 assistive technologies. Each node within the accessibility tree hosts important information about a UI
1015 element. In SCIENCEBOARD, which utilizes an Ubuntu-based GNOME desktop environment, we
1016 employ the Assistive Technology Service Provider Interface ². Specifically, we adopt `pyatspi` to
1017 programmatically retrieve the accessibility tree on Ubuntu.

1018 To make complex `allytree` tractable, and critically, to ensure they fit within the context length
1019 of open-source models, we filter out non-essential elements. This filtering is performed based on
1020 element attributes such as their tag, visibility, and availability. For the elements that remain after
1021 filtering, only key information—specifically their tag, name, text, position, and size—is retained and
1022 subsequently concatenated to form the input representation for the agent.

1023
1024
1025 ²<https://docs.gtk.org/atspi2/>

1026
 1027 **Screenshot + a11ytree.** To further enhance the action execution capabilities of computer-using
 1028 agents, especially for models with weaker grounding abilities, we utilize a combined input of
 1029 screenshots and a11ytree.

1030 **Set-of-Mark.** We follow the official implementation of Set-of-Mark (Yang et al., 2023). We
 1031 leverage the information from the filtered a11ytree and mark the elements on the screenshot with
 1032 a numbered bounding box. Following VisualWebArena (Koh et al., 2024) and UFO (Zhang et al.,
 1033 2024), we further combine the annotated screenshot with the text metadata from a11ytree.

1034

1035 C ACCESSING SCIENCEBOARD ENVIRONMENT

1036
 1037 To facilitate broader adoption and reproducibility, we provide several methods for accessing SCI-
 1038 ENCEBOARD environment. Researchers can choose the most suitable option based on their technical
 1039 requirements and resources:

1040
 1041 **Direct Deployment.** The entire framework, including all scientific software and evaluation scripts,
 1042 is available for direct deployment on a native Ubuntu system. Full setup instructions and dependency
 1043 lists are provided in our repository.

1044

1045 **Docker Container.** We also provide a Docker image that encapsulates the environment, making it
 1046 easy to run SCIENCEBOARD across different machines and operating systems, which is available at
 1047 <https://anonymous.4open.science/r/ScienceBoard/>.

1048

1049 **Cloud Platforms.** For scalability and powerful computational resources, SCIENCEBOARD can be
 1050 deployed on cloud platforms like Amazon Web Services (AWS). We will provide guidelines upon
 1051 acceptance.

1052

1053 D DETAILS OF SCIENCEBOARD BENCHMARK

1054 D.1 TASK ANNOTATION

1055 During the task annotation process, we primarily utilize the tutorials and handbooks listed in Table 6
 1056 to guide annotators in exploring the relevant domain and corresponding software and tools. All app
 1057 data collection and task creation are completed by the authors.

1058

1059 D.2 TASK DIVERSITY

1060 To explore the diversity of tasks in SCIENCEBOARD, we perform a t-SNE (van der Maaten & Hinton,
 1061 2008) visualization, as shown in Figure 6. We obtain embeddings for all task instructions using
 1062 text-embedding-3-small and then apply t-SNE to reduce their dimensionality to two for
 1063 visualization. The semantic distribution of instructions clearly distinguishes tasks across different
 1064 domains, while also revealing considerable diversity within each individual domain. Furthermore,
 1065 we can observe some intersections between Scientific Documentation tasks and tasks from other
 1066 domains, which reflects the presence of cross-application workflows in our benchmark.

1067

1068 D.3 COMPARISON WITH EXISTING BENCHMARKS

1069 We compare SCIENCEBOARD with existing well-established benchmarks for scientific tasks, as
 1070 shown in Table 7.

1071 SCIENCEBOARD is the first to offer a realistic environment for evaluating scientific tasks. In terms of
 1072 I/O, it incorporates structured code input and visual information, which are critical for simulating
 1073 scientific experiment workflows. It also supports GUI automation, making it well-suited for visual
 1074 agents to fulfill tasks like humans do. Additionally, SCIENCEBOARD covers a broader range of task
 1075 types compared to existing works, including but not limited to question-answering and scientific
 1076 computing. These unique features make SCIENCEBOARD both a versatile playground and an
 1077 expandable framework for evaluating agents' scientific capabilities.

Table 6: Sources of the tutorials and handbooks employed in the task annotation process.

Software	Tutorial & Handbook Sources
Kalgebra	https://docs.kde.org/stable5/en/kalgebra/kalgebra/index.html
ChimeraX	https://www.cgl.ucsf.edu/chimerax/tutorials.html https://kpwulab.com/wp-content/uploads/2022/04/chimerax-tutorial-kpwulab-2022-0429.pdf
Lean 4	https://lean-lang.org/theorem_proving_in_lean4/ https://leanprover-community.github.io/mathematics_in_lean/index.html https://lean-lang.org/doc/reference/latest/
Grass GIS	https://grass.osgeo.org/grass84/manuals/index.html https://neteler.gitlab.io/grass-gis-analysis/
Celestia	https://celestiaproject.space/guides.html https://en.wikibooks.org/wiki/Celestia https://celestiaproject.space/docs/CELScriptingGuide/Cel_Script_Guide_v1_0g.htm
TeXStudio	https://texstudio-org.github.io/getting_started.html https://latex-tutorial.com/tutorials/

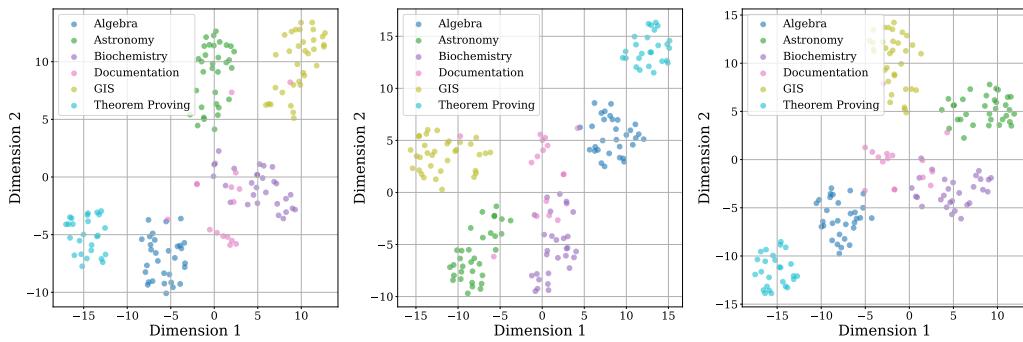


Figure 6: t-SNE visualization of task instructions distribution. The seeds of t-SNE are randomly sampled for each plot.

1134	Feature	SCIENCEBOARD (our work)	ScienceQA (Lu et al., 2022)	SciCode (Tian et al., 2024)	ScienceAgentBench (Chen et al., 2025)
1135	<i>I/O Formats</i>				
1136	Code / Structured Input	✓	✗	✓	✓
1137	Visual Information	✓	✓	✗	✗
1138	<i>Task Type</i>				
1139	Question-Answering	✓	✓	✗	✗
1140	Scientific Computing	✓	✗	✓	✓
1141	GUI Automation	✓	✗	✗	✗

Table 7: A comparison of SCIENCEBOARD to notable and recent AI4Science benchmarks.

D.4 MORE EVALUATION SCRIPT EXAMPLES

Beyond the evaluation cases listed in Section 3.2, Table 8 showcases a broader variety of evaluation pipelines created using our templates.

Table 8: More evaluation cases of SCIENCEBOARD include exact matching, range-based assessment, and numerical tasks with tolerance.

1152	Initial State	Instruction	Evaluation Script (Simplified)
1153		Select all ligand(s) and color them into magenta in ChimeraX.	{ "type": "info", "key": "sel", "value": ["atom id /A:9@N1 idatm_type N3+", ...], "cmd": "v.set_color /A", "key": "sel", "value": ["#1/A:1 color #d2b48c", ...] }
1154			
1155			
1156			
1157			
1158			
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1160			
1161		There is a point located in the Mediterranean Sea. Please find and delete it.	{ "cmd": "v.to.db", "key": "sel", "value": ["point"], "pred": "lambda key, value: key == value" } { "cmd": "db", "key": "sel", "value": ["point"], "pred": "lambda key, value: key == value" }
1162			
1163			
1164			
1165			
1166			
1167			
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1169			
1170		Approach to the Earth and display a solar eclipse in Celestia.	{ "cmd": "v.set_color /A", "key": "sel", "value": "#d2b48c", "pred": "lambda key, value: key == value" } { "cmd": "db", "key": "sel", "value": ["point"], "pred": "lambda key, value: key == value" }
1171			
1172			
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1177			
1178			
1179			
1180			
1181	 theorem TP_3 [TopologicalSpace X] [TopologicalSpace Y] (f : X → Y) (Z : Set X) (h ₁ : Continuous f) (h ₂ : IsConnected Z) : IsConnected {y : Y $\exists z \in Z, f z = y$ } := by sorry		{ "cmd": "info", "key": "sel", "value": ["atom id /A:9@N1 idatm_type N3+", ...], "cmd": "v.set_color /A", "key": "sel", "value": ["#1/A:1 color #d2b48c", ...] }
1182			
1183			
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1187			

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D.5 HUMAN PERFORMANCE

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In our main experiments, as reflected in Table 3, we recruit college-level students to establish normal human performance on SCIENCEBOARD benchmark. Before attempting the tasks, participants are required to familiarize themselves with foundational knowledge of the relevant scientific disciplines and study the provided operational manuals. They were then given instructions, as shown in Instruction 1, to complete the assigned tasks. Participants were compensated at a rate of \$10 per hour for their involvement.

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The SCIENCEBOARD environment and scientific software used do not record any personal information, and all participants provide informed consent. The experiment does not involve surveys, interviews, or any behavioral tracking.

1199

D.6 STABILITY ANALYSIS

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Considering that dynamic environments could potentially lead to experimental instability, we conduct an additional set of experiments focusing on consistency. For these, we utilize GPT-4o under the allytree + screenshot setting, with results and error bars reported in Figure 7.

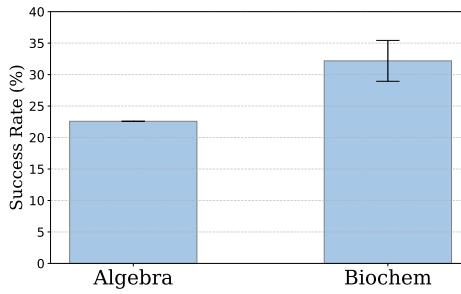
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Figure 7: Stability analysis.

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Across three independent runs, performance on Algebra tasks remains stable. However, Biochemistry tasks exhibited minor fluctuations in success rates. Upon closer inspection of individual cases, we hypothesize that these variations likely stem from network connectivity issues or transient system lag encountered during task execution.

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D.7 EVALUATION COST

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We use API keys to access proprietary models. On average, a single run on all SCIENCEBOARD tasks costs \$64 using GPT-4o, \$86 using Claude-3.7-Sonnet, and \$45 using Gemini-2.0-Flash.

1227

E DETAILS OF EXPERIMENTS

1228
1229

E.1 BACKBONE MODELS

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We briefly discuss the backbones we used to build our computer-using agents.

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Proprietary Models. Proprietary models now demonstrate striking capabilities in complex reasoning and are increasingly exhibiting agentic potential for dynamic real-world interaction, prompting a closer look at their diverse forms. In the experimental section, we accessed the following proprietary models via API keys:

1238
1239
1240
1241

- GPT-4o (Hurst et al., 2024).
- Claude-3.7-Sonnet (Anthropic AI, 2024).
- Gemini-2.0-Flash (Team, 2024).
- o3-mini (OpenAI, 2025).

1242 **Open-source Models.** Open-source models are demonstrating remarkable advancements, steadily
 1243 narrowing the performance gap with proprietary models. Crucially, the open-source community
 1244 recognized the significance of agentic capabilities early on, fostering development in this direction.
 1245 This foresight has translated into exceptional performance, particularly within GUI scenarios where
 1246 these models now excel on various challenging benchmarks. Our evaluation is based on the following
 1247 open-source models, which are characterized by their advanced grounding capabilities:

- 1248 • Qwen2.5-VL-72B-Instruct (Bai et al., 2025): The latest evolution in the Qwen vision-language
 1249 model family, primarily distinguished by its robust agentic capabilities. It operates directly as a
 1250 visual agent, proficient in reasoning, dynamically utilizing tools, and executing tasks for computer
 1251 and phone operation. Complementing its agentic prowess, Qwen2.5-VL-72B-Instruct demonstrates
 1252 advanced proficiency in detailed visual analysis (including texts, charts, icons, and layouts within
 1253 images), comprehension of videos exceeding one hour with event pinpointing, precise object
 1254 localization with structured coordinate output, and the generation of structured data from documents
 1255 such as invoices and forms. In our experiments, this model is deployed using interconnected clusters
 1256 of $8 \times$ A100 80GB GPUs with vLLM (Kwon et al., 2023).
- 1257 • InternVL3-78B (Chen et al., 2024): An advanced MLLM recognized for its superior overall perfor-
 1258 mance and significantly enhanced multimodal perception and reasoning. A key advancement is its
 1259 robust agentic functionality, demonstrated through proficient tool usage and GUI agent operations,
 1260 alongside extended capabilities in areas like industrial image analysis and 3D vision perception.
 1261 These comprehensive abilities are underpinned by innovations such as a native multimodal pre-
 1262 training approach, supervised fine-tuning with diverse, high-quality data tailored to these advanced
 1263 tasks, and mixed preference optimization for refined reasoning. In our experiments, this model is
 1264 deployed using interconnected clusters of $8 \times$ A100 80GB GPUs with vLLM.
- 1265 • QvQ-72B-Preview (Qwen Team, 2024): An experimental research model focused on advancing
 1266 visual reasoning capabilities. It has achieved compelling performance in complex multidisciplinary
 1267 understanding and problem-solving, highlighting its specialized strength in sophisticated visual
 1268 cognitive tasks. However, it exhibits some limitations in instruction following, appearing less adept
 1269 in agent scenarios that require precise action outputs. In our experiments, this model is deployed
 1270 using interconnected clusters of $8 \times$ A100 80GB GPUs with vLLM.

1271 **GUI Action Models.** While foundational models provide impressive general-purpose intelligence,
 1272 their intrinsic agentic capabilities for nuanced GUI manipulation are still under active exploration,
 1273 often requiring further specialization. Consequently, a prominent line of research involves adapting
 1274 open-source VLMs by fine-tuning them on extensive, GUI-specific datasets. This targeted training
 1275 methodology yields dedicated action models equipped with significantly enhanced proficiencies
 1276 for understanding and interacting with GUIs. The GUI action models adopted in this paper are as
 1277 follows:

- 1278 • OS-Atlas-Pro-7B (Wu et al., 2025b): A foundational GUI action model that significantly advances
 1279 open-source VLMs for agentic tasks, excelling in GUI grounding and out-of-distribution scenarios
 1280 through innovations in modeling and the creation of the largest open-source, cross-platform GUI
 1281 grounding corpus with over 13 million elements. It demonstrates state-of-the-art performance
 1282 across six diverse benchmarks (mobile, desktop, web) and verifies the existence of model scaling
 1283 laws in GUI scenarios. In our experiments, this model is deployed using a single A100 80GB GPU
 1284 with vLLM (Kwon et al., 2023).
- 1285 • UGround-V1-7B (Gou et al., 2025): A universal visual grounding model that identifies GUI action
 1286 elements by pixel coordinates. It powers the SeeAct-V framework (Zheng et al., 2024), which
 1287 enables purely visual GUI perception and pixel-level operations. Agents using SeeAct-V with
 1288 UGround have achieved SOTA results across five distinct benchmarks spanning web, mobile, and
 1289 desktop evaluations. In our experiments, this model is deployed on a single A100 80GB GPU with
 1290 vLLM.
- 1291 • UI-TARS-72B-DPO (Qin et al., 2025): An end-to-end native GUI agent that uniquely perceives
 1292 screenshots as its sole input to perform human-like keyboard and mouse interactions, outperforming
 1293 prevailing agent frameworks that depend on heavily wrapped commercial models with expert-
 1294 crafted prompts. It has established state-of-the-art performance across more than ten GUI agent
 1295 benchmarks. This advanced capability stems from key innovations including enhanced perception,
 1296 unified action modeling, System-2 reasoning, iterative training with reflective online traces, and

1296 a final Direct Preference Optimization (DPO) phase, which refines its ability to make precise,
 1297 context-aware decisions. In our experiments, UI-TARS-72B-DPO utilizes vLLM for inference and
 1298 is deployed on interconnected clusters of $8 \times$ A100 80GB GPUs.

1299 • GUI-Actor-7B (Wu et al., 2025a): A recently proposed GUI grounding model that introduces a
 1300 novel coordinate-free visual grounding approach. It utilizes an action head to direct the special
 1301 token <ACTOR> to the target screenshot patches for localization. It claims to surpass the text-based
 1302 coordinate prediction baseline and demonstrates better generalization in out-of-distribution (OOD)
 1303 scenarios. In our experiments, we used the 7B version of GUI-Actor based on the Qwen2.5-VL
 1304 backbone.

1305 **E.2 EVALUATION SETTINGS - MAIN EXPERIMENTS**

1306 We adhered to common prompt engineering strategies from previous works (Sun et al., 2024b; Zhou
 1307 et al., 2024; Zhang & Zhang, 2024) for the agents under evaluation. For each domain, the agent
 1308 interacts with the environment under the guidance of a meta-prompt, which includes information
 1309 about the software being operated, executable special actions, and related details. When taking
 1310 actions, the agent generates outputs in the ReAct style (Yao et al., 2023), with its step-by-step
 1311 thoughts recorded in the interaction history.

1312 Throughout the evaluation, we set the `temperature` parameter to 0.5, `top_p` to 0.9, and
 1313 `max_tokens` to 1500. We list some prompt examples in Prompt 14, Prompt 15, Prompt 16 and
 1314 Prompt 17.

1315 **E.3 EVALUATION SETTINGS - ANALYSIS**

1316 In experiments with interleaved planning and action, we first address inconsistencies in coordinate
 1317 outputs from different GUI action models. While InternVL3-78B (Chen et al., 2024) outputs
 1318 coordinates on a $[0, 1]$ scale, models such as OS-Atlas, UI-TARS, and UGround use a $[0, 1000]$ scale.
 1319 To ensure uniformity, we normalized all coordinate outputs to a $[0, 1]$ scale prior
 1320 to execution.

1321 This part of the experiments employs a two-stage process: First, the planner model receives the
 1322 current observation (`obs`) and task instruction to generate a high-level plan or a specific action. If the
 1323 planner outputted a directly executable primitive action (e.g., a non-GUI system-level command or a
 1324 special control token like `DONE`), that action will be performed immediately, and the action model
 1325 was not invoked for that step. Otherwise, the grounding model received the current observation and
 1326 the plan (or sub-task) from the planner. Its role was to output low-level executable instructions. If
 1327 the grounding model generate `pyautogui` actions directly, these commands were executed. For
 1328 models outputting in their specific native formats, we implement custom parsers to translate these
 1329 into `pyautogui` actions: for UGround and UI-TARS, all coordinate-based outputs were interpreted
 1330 as `click`, whereas for OS-Atlas, its outputs were parsed to differentiate between `click`, `type`,
 1331 and `scroll` based on its defined schema.

1332 We list some prompt examples in Prompt 18, Prompt 19, Prompt 20 and Prompt 21.

1333 **F EXTENDED ANALYSIS**

1334 **F.1 INTERFACES**

1335 In Section 6, we analyze the performance difference between Vision-Only and Hybrid Interface
 1336 settings under the `allytree + screenshot`. Here, we present empirical results under the other three
 1337 observation settings.

1338 As shown in Figure 8, the hybrid GUI + CLI setting consistently achieves performance that is
 1339 comparable to or better than the GUI-Only setting across all scenarios. Interestingly, while GPT-4o
 1340 achieves state-of-the-art performance under other observation settings, it exhibits very weak action
 1341 capabilities when using screenshot setting, indicating the reliance on structured observations for
 1342 effective reasoning and planning.

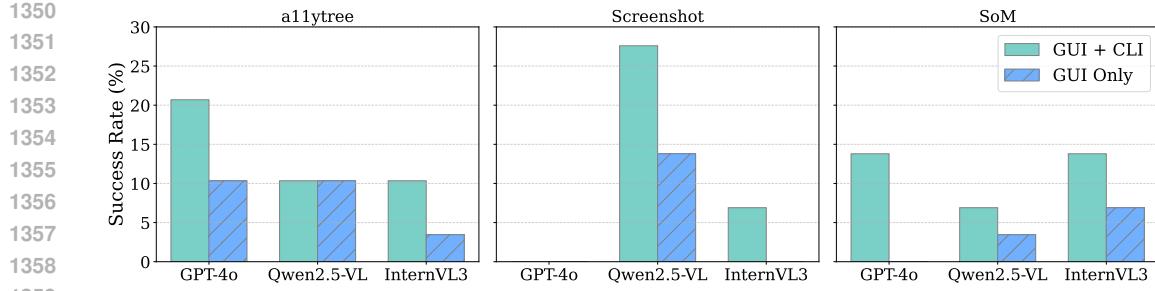


Figure 8: Extended analysis of Vision-Only vs. Hybrid Interface.

F.2 INTERACTIVE ENVIRONMENTS

ATP represents one of the most logic-intensive tasks for agents and has been traditionally studied in textual settings in prior works (*e.g.*, plain text or bash terminal).

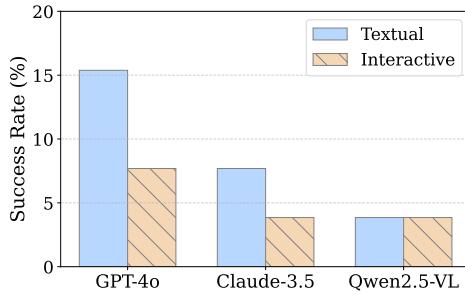


Figure 9: Textual v.s. Interactive

We extend ATP to live OS in SCIENCEBOARD and further compare agents' performance under textual and interactive settings. The latter, similar to environments commonly used by humans, provides a live VSCode interface with features such as syntax highlighting, autocompletion, type inference, and other functionalities. As shown in Figure 9, in the textual setting, the agent applies heuristic strategies (*e.g.*, Monte Carlo search) to make predictions over the proof tree without interacting with the environment. In contrast, in the interactive setting, the agent must autonomously decide which PROOFSTATE to proceed with. Moreover, the agent is also required to localize the relevant code segments within the interface. Completing formal methods tasks becomes substantially more challenging in realistic environments, which significantly increases the cognitive complexity.

F.3 DIFFICULTY ANALYSIS

We further analyze the success rates of computer-using agents on the SCIENCEBOARD benchmark across different task difficulty levels. We employ Claude-3.7-Sonnet, GPT-4o, and Qwen2.5-VL, with results presented in Figure 10.

The findings indicate that solvable tasks are primarily concentrated among a subset of “Easy” problems and a few “Medium” tasks. All “hard” tasks, which involve complex computations, cross-application workflows, or long-horizon planning, could not be completed by any of the evaluated agents.

F.4 FAILURE ANALYSIS

To further investigate the reasons why computer-using agents fail when planning or taking actions on scientific tasks, here we include and discuss several typical examples of such errors.

Opening the Wrong File. This error is frequently caused by grounding issues. The agent initially clicks on an incorrect file and then attempts to perform subsequent actions, such as inputting data,

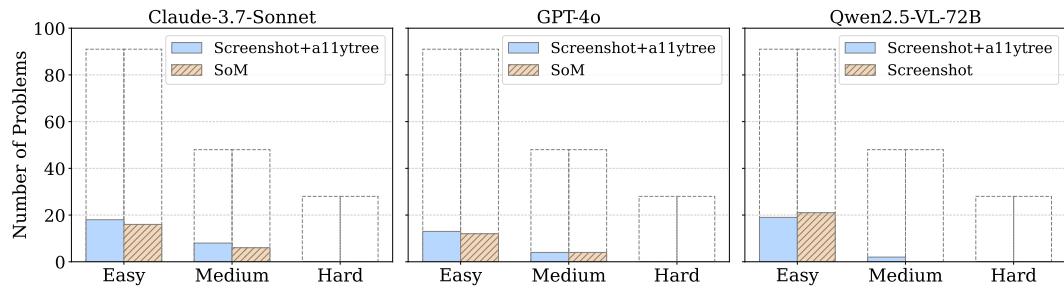


Figure 10: Comparative analysis of task difficulty solve rates.

within that wrong file. This often leads to the agent repeatedly making the same mistake or getting stuck in an unproductive loop. A typical case is shown in Figure 11.

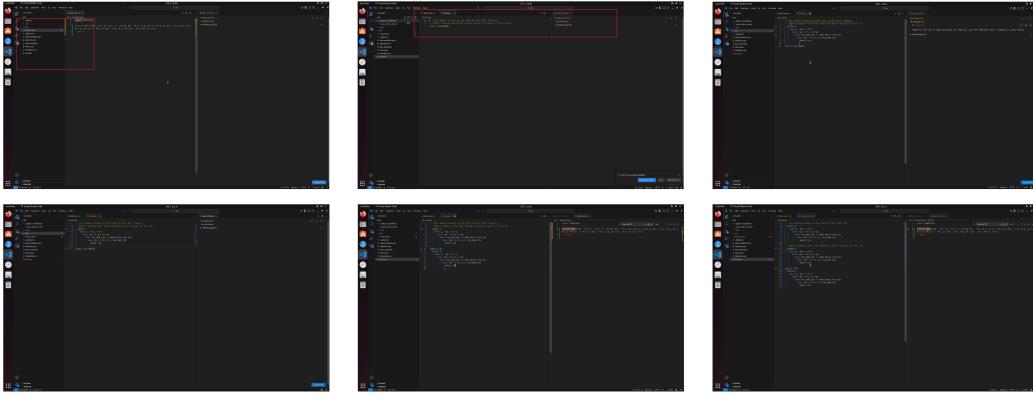


Figure 11: Use wrong file.

Inability to Invoke the Correct Function. In some instances, agents need to identify and use a specific function within a software application but attempt to do so by directly typing an assumed function name into a search bar or command input. If the exact function name is unknown or guessed incorrectly, a more robust strategy would be to browse available menus or function lists. Instead, agents may incorrectly assume knowledge of the function name and attempt to look up its usage, leading to failure. A typical example of this behavior is presented in Figure 12.

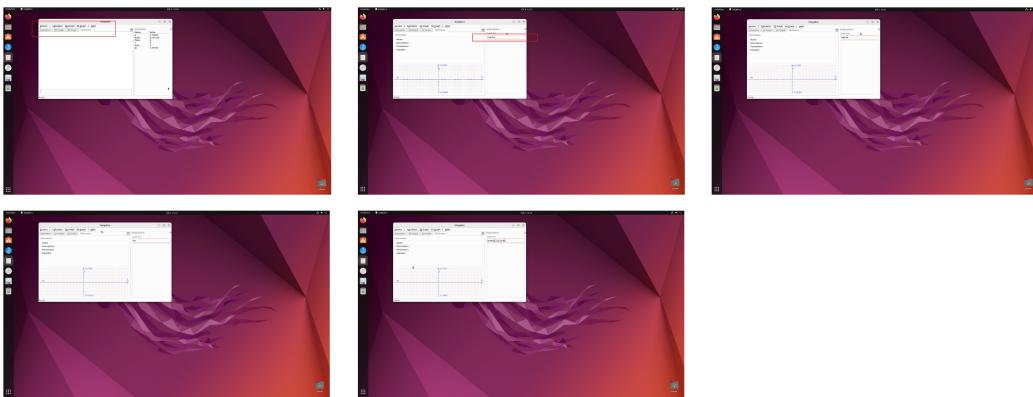


Figure 12: Function invocation error.

Incorrect CLI Code. Failures also occur when agents formulate CLI commands incorrectly. This can involve syntax errors, wrong command names, or incorrect parameters. Notably, in some of

1458 these failed CLI attempts, the intended task could have been accomplished more straightforwardly
 1459 by interacting with a corresponding button or element in the GUI. A typical example is shown in
 1460 Figure 13.

1461

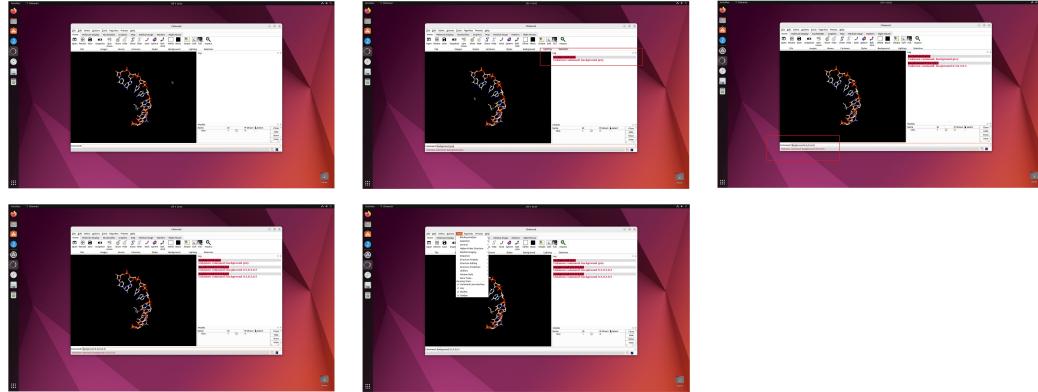


Figure 13: CLI code error.

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G PROMPTS

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The prompt examples we used in SCIENCEBOARD are listed below.

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 1517 **Agentic Prompt - ChimeraX with screenshot**
 1518
 1519 You are an agent which follow my instruction and perform desktop computer
 1520 tasks as instructed.
 1521 You have good knowledge of ChimeraX, a molecular visualization software;
 1522 and assume your code will run on a computer controlling the mouse and
 1523 keyboard.
 1524 For each step, you will get an observation of the desktop by an
 1525 accessibility tree, which is based on AT-SPI library, and you will
 1526 predict actions of the next step based on that.
 1527
 1528 You are required to use 'pyautogui' to perform the action grounded to the
 1529 observation, but DO NOT use the 'pyautogui.locateCenterOnScreen' function
 1530 to locate the element you want to operate with since we have no image of
 1531 the element you want to operate with. DO NOT USE 'pyautogui.screenshot()'`
 1532 to make screenshot.
 1533 You ONLY need to return the code inside a code block, like this:
 1534 ``
 1535 # your code here
 1536 ``
 1537 Return one line or multiple lines of python code to perform the action
 1538 each time, and be time efficient. When predicting multiple lines of
 1539 code, make some small sleep like 'time.sleep(0.5);' interval so that the
 1540 machine could take breaks. Each time you need to predict a complete code,
 1541 and no variables or function can be shared from history.
 1542
 1543 Specially, it is also allowed to return the following special code:
 1544 When you think the task is done, return "DONE";
 1545 When you think the task can not be done, return "FAIL". Don't easily
 1546 say "'FAIL'; try your best to do the task;
 1547 When you think you have to wait for some time, return "WAIT" or "WAIT
 1548 n", in which n defaults to 5(s);
 1549 When you are asked to submit an answer, return "ANS s" without
 1550 quotation marks surrounding s, and use 'FAIL' if there is no answer to
 1551 the question.
 1552
 1553 My computer's password is 'password', feel free to use it when you need
 1554 sudo rights.
 1555 DO NOT introduce any unrelated models or easily close existing models,
 1556 otherwise the task might be evaluated as FAILED.
 1557 DO NOT close the current ChimeraX session, or every effort you made will
 1558 be in vain.
 1559 NEVER try to reopen the command line interface in ChimeraX if it is
 1560 hidden, because it has been deactivated and cannot do anything. But you
 1561 are welcome to use it once it is presented.
 1562
 1563 First give the current observation and previous things we did a short
 1564 reflection, then RETURN ME THE CODE OR SPECIAL CODE I ASKED FOR. NEVER
 1565 EVER RETURN ME ANYTHING ELSE.
 1566 You are asked to complete the following task: Fetch 2OLX from PDB in
 1567 ChimeraX.

1568 **Prompt 14: Prompts for ChimeraX with screenshot**
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 1573 **Agentic Prompt - Celestia with screenshot**
 1574
 1575 You are an agent which follow my instruction and perform desktop computer
 1576 tasks as instructed.
 1577 You have good knowledge of Celestia, a three-dimension space simulator;
 1578 and assume your code will run on a computer controlling the mouse and
 1579 keyboard.
 1580 For each step, you will get an observation of the desktop by a screenshot,
 1581 and you will predict actions of the next step based on that.
 1582
 1583 You are required to use 'pyautogui' to perform the action grounded to the
 1584 observation, but DO NOT use the 'pyautogui.locateCenterOnScreen' function
 1585 to locate the element you want to operate with since we have no image of
 1586 the element you want to operate with. DO NOT USE 'pyautogui.screenshot()' '
 1587 to make screenshot.
 1588 You ONLY need to return the code inside a code block, like this:
 1589 ``
 1590 # your code here
 1591 ``
 1592 Return one line or multiple lines of python code to perform the action
 1593 each time, and be time efficient. When predicting multiple lines of
 1594 code, make some small sleep like 'time.sleep(0.5);' interval so that the
 1595 machine could take breaks. Each time you need to predict a complete code,
 1596 and no variables or function can be shared from history.
 1597
 1598 Specially, it is also allowed to return the following special code:
 1599 When you think the task is done, return "DONE";
 1600 When you think the task can not be done, return "FAIL". Don't easily
 1601 say "FAIL"; try your best to do the task;
 1602 When you think you have to wait for some time, return "WAIT" or "WAIT
 1603 n", in which n defaults to 5(s);
 1604 When you are asked to submit an answer, return "ANS s" without
 1605 quotation marks surrounding s, and use 'FAIL' if there is no answer to
 1606 the question.
 1607
 1608 My computer's password is 'password', feel free to use it when you need
 1609 sudo rights.
 1610 The criterion for a celestial body to be displayed on the screen is that
 1611 the object's center is within the window range and is not blocked by
 1612 others.
 1613 First give the current observation and previous things we did a short
 1614 reflection, then RETURN ME THE CODE OR SPECIAL CODE I ASKED FOR. NEVER
 1615 EVER RETURN ME ANYTHING ELSE.
 1616 You are asked to complete the following task: Set the Julian date to
 1617 2400000 in Celestia.
 1618
 1619

Prompt 15: Prompts for Celestia with screenshot

1620 **Agentic Prompt - ChimeraX with set-of-marks**
 1621
 1622 You are an agent which follow my instruction and perform desktop computer
 1623 tasks as instructed.
 1624 You have good knowledge of ChimeraX, a molecular visualization software;
 1625 and assume your code will run on a computer controlling the mouse and
 1626 keyboard.
 1627 For each step, you will get an observation of the desktop by 1) an
 1628 accessibility tree, which is based on AT-SPI library; and 2) a screenshot
 1629 with interactable elements marked with numerical tags, and you will
 1630 predict actions of the next step based on that.
 1631
 1632 You are required to use 'pyautogui' to perform the action grounded to the
 1633 observation, but DO NOT use the 'pyautogui.locateCenterOnScreen' function
 1634 to locate the element you want to operate with since we have no image of
 1635 the element you want to operate with. DO NOT USE 'pyautogui.screenshot()' to
 1636 make screenshot.
 1637 You ONLY need to return the code inside a code block, like this:
 1638 ``
 1639 # your code here
 1640 ``
 1641 Return one line or multiple lines of python code to perform the action
 1642 each time, and be time efficient. When predicting multiple lines of
 1643 code, make some small sleep like 'time.sleep(0.5);' interval so that the
 1644 machine could take breaks. Each time you need to predict a complete code,
 1645 and no variables or function can be shared from history.
 1646
 1647 You can replace x, y in the code with the tag of elements you want to
 1648 operate with, such as:
 1649 ``
 1650 pyautogui.moveTo(tag_3)
 1651 pyautogui.click(tag_2)
 1652 pyautogui.dragTo(tag_1, button='left')
 1653 ``
 1654 When you think you can directly output precise x and y coordinates or
 1655 there is no tag on which you want to interact, you can also use them
 1656 directly; but you should be careful to ensure the correct of coordinates.
 1657
 1658 Specially, it is also allowed to return the following special code:
 1659 When you think the task is done, return "DONE";
 1660 When you think the task can not be done, return "FAIL". Don't easily
 1661 say "FAIL"; try your best to do the task;
 1662 When you think you have to wait for some time, return "WAIT" or "WAIT
 1663 n", in which n defaults to 5(s);
 1664 When you are asked to submit an answer, return "ANS s" without
 1665 quotation marks surrounding s, and use 'FAIL' if there is no answer to
 1666 the question.
 1667
 1668 My computer's password is 'password', feel free to use it when you need
 1669 sudo rights.
 1670 DO NOT introduce any unrelated models or easily close existing models,
 1671 otherwise the task might be evaluated as FAILED.
 1672 DO NOT close the current ChimeraX session, or every effort you made will
 1673 be in vain.
 1674 NEVER try to reopen the command line interface in ChimeraX if it is
 1675 hidden, because it has been deactivated and cannot do anything. But you
 1676 are welcome to use it once it is presented.
 1677
 1678 First give the current observation and previous things we did a short
 1679 reflection, then RETURN ME THE CODE OR SPECIAL CODE I ASKED FOR. NEVER
 1680 EVER RETURN ME ANYTHING ELSE.
 1681 You are asked to complete the following task: Fetch 2OLX from PDB in
 1682 ChimeraX.
 1683

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 1675
 1676 **Agentic Prompt - Celestia with set-of-marks**
 1677
 1678 You are an agent which follow my instruction and perform desktop computer
 1679 tasks as instructed.
 1680 You have good knowledge of Celestia, a three-dimension space simulator;
 1681 and assume your code will run on a computer controlling the mouse and
 1682 keyboard.
 1683 For each step, you will get an observation of the desktop by 1) an
 1684 accessibility tree, which is based on AT-SPI library; and 2) a screenshot
 1685 with interact-able elements marked with numerical tags, and you will
 1686 predict actions of the next step based on that.
 1687
 1688 You are required to use 'pyautogui' to perform the action grounded to the
 1689 observation, but DO NOT use the 'pyautogui.locateCenterOnScreen' function
 1690 to locate the element you want to operate with since we have no image of
 1691 the element you want to operate with. DO NOT USE 'pyautogui.screenshot()' '
 1692 to make screenshot.
 1693 You ONLY need to return the code inside a code block, like this:
 1694 ``
 1695 # your code here
 1696 ``
 1697 Return one line or multiple lines of python code to perform the action
 1698 each time, and be time efficient. When predicting multiple lines of
 1699 code, make some small sleep like 'time.sleep(0.5);' interval so that the
 1700 machine could take breaks. Each time you need to predict a complete code,
 1701 and no variables or function can be shared from history.
 1702
 1703 You can replace x, y in the code with the tag of elements you want to
 1704 operate with, such as:
 1705 ``
 1706 pyautogui.moveTo(tag_3)
 1707 pyautogui.click(tag_2)
 1708 pyautogui.dragTo(tag_1, button='left')
 1709 ``
 1710 When you think you can directly output precise x and y coordinates or
 1711 there is no tag on which you want to interact, you can also use them
 1712 directly; but you should be careful to ensure the correct of coordinates.
 1713
 1714 Specially, it is also allowed to return the following special code:
 1715 When you think the task is done, return "DONE";
 1716 When you think the task can not be done, return "FAIL". Don't easily
 1717 say "FAIL"; try your best to do the task;
 1718 When you think you have to wait for some time, return "WAIT" or "WAIT
 1719 n", in which n defaults to 5(s);
 1720 When you are asked to submit an answer, return "ANS s" without
 1721 quotation marks surrounding s, and use 'FAIL' if there is no answer to
 1722 the question.
 1723
 1724 My computer's password is 'password', feel free to use it when you need
 1725 sudo rights.
 1726 The criterion for a celestial body to be displayed on the screen is that
 1727 the object's center is within the window range and is not blocked by
 1728 others.
 1729
 1730 First give the current observation and previous things we did a short
 1731 reflection, then RETURN ME THE CODE OR SPECIAL CODE I ASKED FOR. NEVER
 1732 EVER RETURN ME ANYTHING ELSE.
 1733 You are asked to complete the following task: Set the Julian date to
 1734 2400000 in Celestia.

1725 Prompt 17: Prompts for Celestia with Set-of-Marks
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Human Instructions

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You are required to finish the given tasks manually to provide sample data of human accuracy.

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First, please start up the evaluation script with debug option ON and headless option OFF. Then, wait for the environment to be initialized and perform your actions when you receive corresponding logs from stdout. Press ENTER after you finish operating and the script will evaluate your result submitted automatically.

1735

Attention:

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1. If you need to finish the task with primitives other than TIMEOUT, please input directly into stdin;
2. You can search for documents or manuals if you encounter domain-specific knowledge you are not familiar with;
3. Make sure that the number of your steps is less than expected. To be more precise, a popup without possibility to predict its position should be split into different steps.

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Instruction 1: Instruction for humans.

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Agentic Prompt - OS-Atlas

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You are an agent which follow my instruction and perform desktop computer tasks as instructed.

1752

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You have good knowledge of Celestia, a three-dimension space simulator; and assume your code will run on a computer controlling the mouse and keyboard.

1754

1755

For each step, you will get an observation of the desktop by a screenshot, together with a plan generated by the planner, and you will parse the plan to operate actions of next steps based on that.

1756

1757

1758

You are required to use your grounding ability to perform the action grounded to the observation and the plan.

1759

1760

You need to return a basic action together with arguments, of which the available ones are listed below:

CLICK: to click at the specified position.

1761

1762

- format: CLICK <point>[[x-axis, y-axis]]</point>
- example usage: CLICK <point>[[101, 872]]</point>

TYPE: to enter specified text at the designated location.

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- format: TYPE [input text]
- example usage: TYPE [Shanghai shopping mall]

SCROLL: to scroll in the specified direction.

1765

1766

- format: SCROLL [direction (UP/DOWN/LEFT/RIGHT)]
- example usage: SCROLL [UP]

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My computer's password is 'password', feel free to use it when you need sudo rights.

1769

1770

Some plans provided may contains unexpected code blocks or confusing instructions. Be flexible and adaptable according to changing circumstances.

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1772

First give the current observation and the generated plan, then RETURN ME THE CODE I ASKED FOR. NEVER EVER RETURN ME ANYTHING ELSE.

1773

1774

You are asked to complete the following task: Set the Julian date to 2400000 in Celestia.

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Prompt 18: Prompts for OS-Atlas

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1798 Agentic Prompt - UGround

1799 You are an agent which follow my instruction and perform desktop computer
 1800 tasks as instructed.
 1801 You have good knowledge of Celestia, a three-dimension space simulator;
 1802 and assume your code will run on a computer controlling the mouse and
 1803 keyboard.
 1804 For each step, you will get an observation of the desktop by a screenshot,
 1805 together with a plan generated by the planner, and you will parse the
 1806 plan to operate actions of next steps based on that.
 1807 You are required to use your grounding ability to perform the action
 1808 grounded to the observation and the plan.
 1809 You need to return a 2d coordinate (x, y) indicating the position you
 1810 want to click.
 1811 My computer's password is 'password', feel free to use it when you need
 1812 sudo rights.
 1813 Some plans provided may contains unexpected code blocks or confusing
 1814 instructions. Be flexible and adaptable according to changing
 1815 circumstances.
 1816 First give the current observation and the generated plan, then RETURN
 1817 ME THE CODE I ASKED FOR. NEVER EVER RETURN ME ANYTHING ELSE.
 1818 You are asked to complete the following task: Set the Julian date to
 1819 2400000 in Celestia.

1820 **Prompt 19: Prompts for UGround**
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1843 Agentic Prompt - Qwen

1844 You are an agent which follow my instruction and perform desktop computer
 1845 tasks as instructed.
 1846 You have good knowledge of Celestia, a three-dimension space simulator;
 1847 and assume your code will run on a computer controlling the mouse and
 1848 keyboard.
 1849 For each step, you will get an observation of the desktop by a screenshot,
 1850 together with a plan generated by the planner, and you will parse the
 1851 plan to operate actions of next steps based on that.
 1852
 1853 You are required to use 'pyautogui' to perform the action
 1854 grounded to the observation and the plan, but DO NOT use the
 1855 'pyautogui.locateCenterOnScreen' function to locate the element you want
 1856 to operate with since we have no image of the element you want to operate
 1857 with. DO NOT USE 'pyautogui.screenshot()' to make screenshot.
 1858 You ONLY need to return the code inside a code block, like this:
 1859
 1860 ``
 1861 # your code here
 1862 ``
 1863 Return one line or multiple lines of python code to perform the action
 1864 each time, and be time efficient. When predicting multiple lines of
 1865 code, make some small sleep like 'time.sleep(0.5);' interval so that the
 1866 machine could take breaks. Each time you need to predict a complete code,
 1867 and no variables or function can be shared from history.
 1868
 1869 Specially, it is also allowed to return the following special code:
 1870 When you think the task is done, return "'DONE'";
 1871 When you think the task can not be done, return "'FAIL'". Don't easily
 1872 say "'FAIL"'; try your best to do the task;
 1873 When you think you have to wait for some time, return "'WAIT'" or "'WAIT
 1874 n'", in which n defaults to 5(s);
 1875 When you are asked to submit an answer, return "'ANS s'" without
 1876 quotation marks surrounding s, and use 'FAIL' if there is no answer to
 1877 the question.
 1878
 1879 My computer's password is 'password', feel free to use it when you need
 1880 sudo rights.
 1881 Some plans provided may contains unexpected code blocks or confusing
 1882 instructions. Be flexible and adaptable according to changing
 1883 circumstances.
 1884
 1885 First give the current observation and the generated plan, then RETURN
 1886 ME THE CODE OR SPECIAL CODE I ASKED FOR. NEVER EVER RETURN ME ANYTHING
 1887 ELSE.
 1888 You are asked to complete the following task: Set the Julian date to
 1889 2400000 in Celestia.

1883 **Prompt 20: Prompts for Qwen**

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1907 Agentic Prompt - UI-Tars
 1908 You are an agent which follow my instructions and performs desktop
 computer tasks as instructed.
 1909 You have good knowledge of Celestia, a three-dimension space simulator;
 1910 and assume your code will run on a computer controlling the mouse and
 keyboard.
 1911 For each step, you will get an observation of the desktop by a screenshot,
 1912 together with a plan generated by the planner, and you will parse the
 1913 plan to operate actions of next steps based on that.
 1914
 1915 You are required to use your grounding ability to perform the action
 grounded to the observation and the plan.
 1916 You need to return a 2d coordinate (x, y) indicating the position you
 1917 want to click.
 1918
 1919 My computer's password is 'password', feel free to use it when you need
 sudo rights.
 1920 Some plans provided may contains unexpected code blocks or confusing
 1921 instructions. Be flexible and adaptable according to changing
 1922 circumstances.
 1923
 1924 First give the current observation and the generated plan, then RETURN
 1925 ME THE CODE I ASKED FOR. NEVER EVER RETURN ME ANYTHING ELSE.
 1926 You are asked to complete the following task: Set the Julian date to
 1927 2400000 in Celestia.
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Prompt 21: Prompts for UI-TARS