TUMIX: Multi-Agent Test-Time Scaling with Tool-Use Mixture

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While integrating tools like Code Interpreter and Search has significantly enhanced Large Language Model (LLM) reasoning in models like ChatGPT Agent and Gemini-Pro, practical guidance on optimal tool use is lacking. The core challenge is effectively combining textual reasoning, coding, and search for diverse questions. In this paper, we propose Tool-Use Mixture (TUMIX), an ensemble framework that runs multiple agents in parallel, each employing distinct tool-use strategies and answer paths. Agents in TUMIX iteratively share and refine responses based on the question and previous answers. In experiments, TUMIX achieves significant gains over state-of-the-art tool-augmented and test-time scaling methods, delivering an average accuracy improvement of up to 3.55% over the best baseline on Gemini-2.5-Pro and Gemini-2.5-Flash across key reasoning benchmarks, with near-equal inference costs. We find that agent diversity and quality are crucial and can be enhanced by using LLMs to auto-optimize agent designs. Furthermore, TUMIX can halt refinement upon reaching sufficient confidence, preserving performance at only 49% of the inference cost. Further scaling can achieve higher performance, albeit at a greater cost.
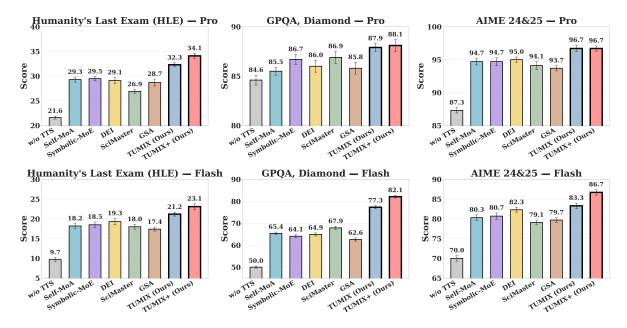

Figure 1 | Comparison of tool-augmented test-time scaling methods on Gemini-2.5-Pro (first row) and Gemini-2.5-Flash (second row) across HLE, GPQA, and AIME 24&25. Except for methods without test-time scaling (`w/o TTS`) or additional scaling (`TUMIX+`), all methods in the same subplot use nearly the same number of inferences and tokens. For fair comparison, methods that originally lacked tool use are run with strong tool-augmented agents instead of text-only agents. Each score is the average of three repetitive runs.

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1. Introduction

While reinforcement learning-based fine-tuning has greatly improved LLM reasoning (Guo et al., 2025), models still struggle with seemingly simple tasks (Chen et al., 2024b). Such tasks are often better handled with code (Madaan et al., 2022; Chen et al., 2022) or search (Jin et al., 2025; Li et al., 2025b). Textual reasoning is strong in semantics and commonsense, but weak in precise computation and in accessing or updating the latest knowledge.

A key challenge is fully utilizing the potential capabilities of textual reasoning, coding, and searching when facing distinctive questions with varied characteristics. Most input questions lack explicit cues for the best approach, and the combined text/code/search solution space is large. Frontier LLM-powered products such as ChatGPT, Claude, Gemini, and Grok report using code and search at test time to augment reasoning, but without publishing detailed methods. Recent work (Chen et al., 2024b) shows that current Code Interpreter implementations in OpenAI models often fail to balance text and code, leaving coding capabilities underused, as shown in Appendix Fig. 11. Moreover, public research still lacks a clear understanding of how to integrate Code Interpreter and Search for improved LLM reasoning.

To better leverage both tool use and LLM self-reasoning, we propose Tool-Use Mixture (TUMIX), a framework that integrates Code Interpreter and Search into LLMs via test-time scaling. TUMIX runs multiple diverse agents in parallel, each with different tool-use strategies. Their outputs are iteratively aggregated and refined across multiple rounds. In each round, every agent generates a new solution by considering both the original question and the previous round's reasoning and answers from all agents. TUMIX uses diverse agents and tool-augmented reasoning strategies to explore a wide range of possible solutions. The following iterative process encourages diverse reasoning paths and deeper integration. This design is inspired by prior test-time scaling methods such as Mixture-of-Agents (MoA) (Wang et al., 2024), which rely on multiple LLMs within a single framework and do not incorporate external tools. In contrast, TUMIX employs a single LLM with both text-only and tool-augmented agent frameworks, making it more generalizable for practical applications. Furthermore, in tool-augmented multi-agent test-time scaling, we find a diverse group of agents outperforms repeated use of the single best agent, a conclusion that differs from MoA (Li et al., 2025a). We later reveal that human pre-designed agent group can be further optimized by querying LLMs to self-design more diverse high-quality agents based on current ones, adding an average 1.2% improvement without cost increase.

Since questions vary in difficulty, they require different amounts of iterative refinement. We query the LLMs to decide whether to terminate refinement early, while still enforcing a minimum number of rounds to maintain answer quality. This adaptive early-termination strategy reduces inference costs to 49% of the original two settings (termination in a fixed round number or by majority-vote consistency across rounds), while preserving or even improving performance. The improvement arises because over-refinement rarely changes the final result and can even degrade performance, as correct answers may be mistakenly discarded.

Compared to the model without test-time scaling, TUMIX delivers an average +7.8% and +17.4% accuracy gains in benchmarks Humanity's Last Exam (HLE) (Phan et al., 2025), Graduate-Level Google-Proof Q&A (GPQA, Diamond) (Rein et al., 2024), and American Invitational Mathematics Examination (AIME 24&25) with base models Gemini-2.5-Pro and Gemini-2.5-Flash, respectively. Under the same inference costs, TUMIX also outperforms existing representative test-time scaling methods such as Self-MoA, Symbolic-MoE, DEI, SciMaster, and GSA, with an average +3.55% lifting compared to the best performing baselines. Notably, with further scaling, TUMIX raises Gemini-2.5-Pro accuracy on HLE from 21.6% to 34.1%, surpassing Gemini-2.5-Pro Deep Research at 26.9% (32.4%

with higher compute) (Comanici et al., 2025). Test-time scaling hinges on two stages (Brown et al., 2024): (1) generating diverse candidate solutions and (2) selecting the correct one. For questions with both small answer spaces (e.g., multiple-choice) and large ones, diverse sampling greatly improves coverage. While it achieves high coverage on HLE (among generated answers in the whole round, at least one is correct on $\geq 65\%$ of questions), accuracy plateaus at about 34% because LLMs struggle to identify the correct answer among noisy candidates. We identify and explore four key factors: agent quality, agent diversity, refinement termination, and answer selection. Our work makes the following contributions:

1. **TUMIX: A competitive tool-augmented test-time scaling method.** We propose TUMIX, a novel framework for test-time scaling that integrates tool augmentation. Extensive experiments demonstrate that TUMIX consistently outperforms strong baselines, achieving an average improvement of +3.55% over the best-performing prior methods.

2. **Key factors and mechanisms in tool-augmented scaling.** We provide a systematic analysis that distinguishes tool-augmented scaling from traditional test-time scaling:

- *Agent diversity and quality outweigh scale alone.* High-temperature sampling increases coverage, but heterogeneous agent strategies yield higher accuracy and lower cost than repeatedly sampling from a single best-performing agent.
- *Tool augmentation boosts performance.* Agent groups equipped with tools such as Code Interpreter and Search achieve superior coverage and accuracy compared to text-only agent groups.

3. **LLMs as agent designers.** We show that prompting LLMs to automatically generate diverse, high-quality agents based on existing ones further improves TUMIX. This yields an additional average accuracy lift of +1.2%.

4. **LLM-as-Judge for refinement termination.** We introduce an LLM-based judge to adaptively determine the optimal stopping round in iterative refinement. This prevents excessive refinement, which reduces diversity and can mistakenly discard correct answers. By enforcing a minimum refinement depth and querying the judge for termination, we achieve near-optimal accuracy while reducing inference cost to ~49% of the original.

2. Related Work

Code Interpreter and Search Many benchmark tasks can in fact be better solved through code (Gao et al., 2023) and search (Li et al., 2025b), and recent work extends coding to reasoning and semantic analysis (Li et al., 2023a; Weir et al., 2024). Most prior approaches use either text (Yao et al., 2024) or code (Bairi et al., 2024; Zhou et al., 2023) exclusively as output. Recent work (Chen et al., 2024b) emphasizes the need to dynamically switch between modalities, proposing CodeSteer (Chen et al.) as a guidance model. Extensions with retrieval (Jin et al., 2025; Li et al., 2025b) and tool use (Qian et al., 2025) further improve reasoning, but lack the thorough exploitation of Code Interpreter and Search tools. Leading models such as OpenAI's ChatGPT Agent, Google's Gemini-Pro (Comanici et al., 2025), and XAI's Grok4 report using code and search at test time to augment reasoning, but without publishing detailed methods. Open work such as ToRL (Li et al., 2025c) and ReTool (Feng et al., 2025) investigates training reasoning models to integrate with Code Interpreters. However, their training and evaluation are limited to math problems, leaving a significant gap from real-world applications that demand effectiveness across broader benchmarks. ToolRL (Qian et al., 2025) instead focuses on teaching models to select among multiple tools, where the generated codes and search queries are relative simple and the evaluation tasks require less reasoning capabilities. SciMaster (Chai et al., 2025) samples the same pre-designed tool-use agent five times, then uses other pre-designed agents

Table 1 | 15 pre-designed agents used in `TUMIX`.

Full Name	Short Name	Description (15 agents)
`w/o TTS`	`Base`	Direct prompt.
`CoT Agent`	`CoT`	Chain-of-Thought prompt (Wei et al., 2022).
`CoT-Code Agent`	`CoT`$_{code}$	CoT prompt to output code.
`Search Agent`	`S`	Uses WebSearch (LLM inherent tool only).
`Code Agent`	`C`	Uses Code Interpreter (base version).
`Code Agent+`	`C`$^+$	Uses Code Interpreter (hinted version with extra human pre-designed priors).
`Dual-Tool Agent`	`CS`	Uses Code Interpreter + WebSearch (with 3 search variants).
`Guided Agent`	`CSG`	Dual-Tool agent (CS) *guided* by a steering module (Chen et al.) (with 3 search variants).
`Guided Agent+`	`CSG`$^+$	*Guided* agent (CSG) with enhanced/hinted prompts (with 3 search variants).

to critique, refine, and aggregate the answers. This approach shows clear improvement over single-inference text-only baselines, but the extent and manner of tool exploitation remain underexplored. In summary, integrating Code Interpreter and Search into LLM reasoning is essential and challenging. The academic community currently lacks methods and studies that fully exploit the benefits of LLM self-reasoning, code execution, and search, which is the focus of our work.

Test-time scaling   LLM self-exploration, reflection, and evaluation can enhance task performance across domains (Yang et al., 2022; Welleck et al., 2022; Madaan et al., 2023). Models like OpenAI o1 (Jaech et al., 2024) and DeepSeek R1 (Guo et al., 2025) showcase agentic behavior via Chain-of-Thought (CoT) reasoning and self-reflection, which is learned by RL-based training with rule-based outcome rewards (Shao et al., 2024; Wei et al., 2025). Apart from the training-based scaling, many research also explore scaling during LLM inference time by pre-designing prompt and agent frameworks. In these works, multi-agent reasoning has emerged as a promising paradigm for enhancing complex problem-solving and decision-making in AI systems (Wu et al., 2023; Li et al., 2023b; Topsakal & Akinci, 2023). Prior work finds gathering the answers from different LLMs improves LLM performance (Du et al.). Mixture-of-Agents (MoA) (Wang et al., 2024) further extends this idea by sharing and gathering answer among LLMs. However, Self-MoA (Li et al., 2025a) argues that LLM diversity may not be critical since replacing different types of LLMs with the best one achieves better performance. Symbolic-MoE (Chen et al., 2025b) further assigns different questions with different specialized LLMs. Instead of using different types of LLMs, many works such as DEI (Zhang et al., 2024), GSA (Li et al., 2025d), and SETS (Chen et al., 2025a) employ different agents from the same LLM for extensive test-time scaling, in which the agent types and frameworks are explored (Chen et al., 2024a). Similar to our work, previous work in test-time scaling also finds the correct answer selection (Brown et al., 2024) is the main bottleneck. While previous work in test-time scaling do not incorporate tool-use of Code Interpreter and Search, we study how to utilize test-time scaling methods to better exploit the benefits of each reasoning mode.

3. Tool-Use Mixture

Appendix B presents the full TUMIX algorithm, and Appendix C lists all agent prompts.

3.1. Pre-designed diverse agents

As shown in Fig. 2, we regard `TUMIX` as sequential decision-making under a compute budget with diverse and correlated experts (agents). Each round selects which agents to run, what they may read (communication policy), when to stop (optimal stopping), and how to aggregate (decision rule), trading off accuracy and cost. Let q be a task with unknown correct answer $a^\star$ in answer space $\mathcal{A}$. There is a pool of agents $\mathcal{S} = \{s_1, \ldots, s_K\}$. Agent s_i outputs an answer $Y_i \in \mathcal{A}$ at cost c_i and
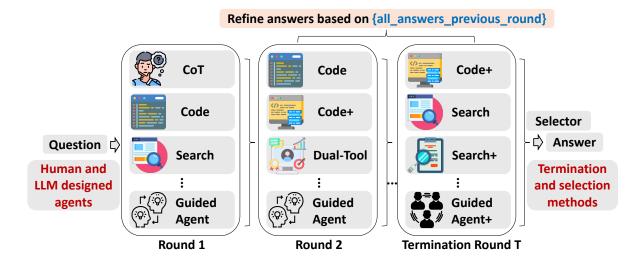
Figure 2 | Overview of TUMIX framework. At each iteration, the responses from all agents in the previous round are concatenated with the original question, forming a joint prompt for the next round. This prompt is then provided to all agents (either the same or new agent groups) to produce refined answers. The subsequent prompts follow the structure illustrated in the above. The design of the agents, their number and specialization, the refinement termination criteria, and the selection strategies are the key factors that determine the effectiveness of the framework.

has competence $p_i(q) = \mathbb{P}\{Y_i = a^\star \mid q\}$. Let $Z_i = \mathbf{1}\{Y_i = a^\star\}$ denote correctness indicators. Their dependencies (and hence ensemble diversity) are captured by a correlation or mutual-information structure over $\{Z_i\}$.

A policy π (our focus) chooses in each round: (i) which agents to run, (ii) the communication graph (what each agent may read from prior rounds), (iii) the stopping rule, and (iv) the aggregation rule producing $\hat{a}_\pi$. A canonical objective is

$$\max_\pi \ \mathbb{P}\{\hat{a}_\pi = a^\star\} \ - \ \lambda \cdot \text{Cost}_\pi, \tag{1}$$

where $\lambda > 0$ trades off compute and accuracy. In our work, the Cost_π is the total number of inference times and input and output tokens to generate the final answer. In the default TUMIX setting, we utilize the same 15 pre-designed agents in all answer refinement rounds. These 15 agents have distinct reasoning and tool-use strategies, as summarized in Table 1. Agents with search access have three search methods (Google Search API (gs), inherent LLM search function (llm), or their combination (com)), yielding three variants per agent. For agents employing multi-round interactions with Search or Code Interpreter, the maximum tool interaction round number is set to 5. In Section 5.3, we discuss how to further query LLMs to automatically optimize and design more diverse agents to achieve better performance. We also compare with a dynamic setting where agent types vary across rounds.

3.2. Refinement as message passing (accuracy rises and diversity shrinks)

In each round, every agent independently generates a new solution by considering both the original question and the solutions provided by all agents in the previous round, as shown in Fig. 2. We evaluate the refinement process using two metrics: average accuracy and coverage (the probability of at least one correct) across agents in each round, which capture the quality and diversity of group answers (Brown et al., 2024). For a set $S \subseteq \mathcal{S}$, the coverage is

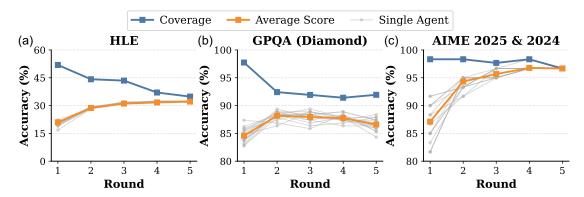$$Coverage(S) = \mathbb{P}\Big(\bigcup_{i \in S}\{Y_i = a^\star\}\Big). \tag{2}$$

Figure 3 | Evolution of coverage, individual agent scores, and average scores across refinement rounds. Coverage decreases monotonically across all benchmarks. For HLE and AIME, the average score rises over the initial rounds before plateauing. For GPQA, the average score improves early on but subsequently declines with further refinement.
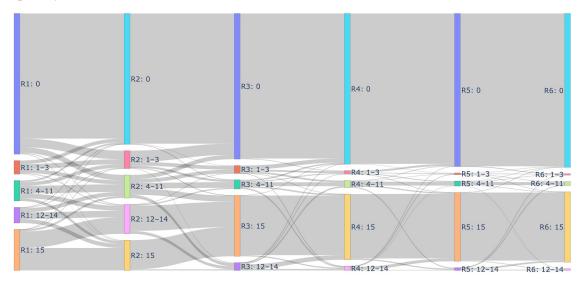

Figure 4 | Sankey diagram of the evolution of correctly answering agents across 2,500 HLE questions over refinement rounds. Based on the distribution dynamics, we define five categories: all wrong (0), few correct (1–3), moderate correct (4–11), high correct (12–14), and all correct (15).

Under independence, $Coverage(S) = 1 - \prod_{i \in S}(1 - p_i)$. With positive correlations, $Coverage(S)$ shrinks. Fig. 3 shows the typical evolution dynamics of coverage, individual agent accuracy, and average scores over refinement rounds. Across all three benchmarks, coverage steadily declines, indicating that some correct answers are mistakenly discarded during iterative refinement. For HLE and AIME, the average score rises in the early rounds and then plateaus, while for GPQA it improves from round 1 to 2 but later declines. Fig. 4 visualizes the dynamics over 2,500 HLE questions. From round 1 to 2, the number of partially correct cases (few/moderate/high correct) increases, while both all wrong and all correct cases decrease. This suggests that initial thought-sharing broadens exploration and promotes diversity. After round 2, however, partially correct cases diminish toward near zero, while all wrong and all correct cases grow. This indicates that agents gradually converge to a single shared answer across rounds, either correct or incorrect.

3.3. Termination in optimal rounds and final answer selection

The observed evolution indicates that round-by-round refinement not only improves answers in the initial rounds but also drives convergence, as each agent selects based on prior responses. However,

due to the limited reasoning ability of LLMs, many correct answers are prematurely discarded. Beyond the early rounds, refinement rarely yields further accuracy gains and, in some cases, even degrades performance. Thus, identifying an effective termination strategy is essential for both robust performance and cost efficiency. Let A_r denote acquired accuracy after round r. Define the expected marginal value of another round

$$\Delta_r = \mathbb{E}[A_{r+1} - A_r \,|\, \text{signals up to round } r]. \tag{3}$$

Stop at the first round r where $\Delta_r \leq \lambda \cdot$ marginal cost (here is increased inference costs). A practical termination strategy decides whether to stop based on the estimated future gain Δ_r, which relies on round-r statistics such as (i) diversity collapse (coverage drop; rising agreement), (ii) vote margin between top answers, and (iii) answer entropy.

In TUMIX, our termination determination strategy is to query the LLM to decide whether to stop refinement and finalize answers based on the current round, with a minimum round number of 2. We find this termination strategy achieves nearly the same performance with only 49% of the inference cost. In Section 5.2, we explore other termination methods such as stopping once the majority answer stabilizes across two consecutive rounds or termination based on LLM confidence scores (Fu et al., 2025), but find only worse performance. After termination, we obtain the final answer through majority voting over the agents' responses, with Gemini-2.5-Pro selecting the most consistent output.

4. Experiments

4.1. Experimental settings

Benchmarks   For a comprehensive evaluation and comparison across methods, we conduct experiments on three representative benchmarks that demand extensive reasoning and planning, particularly the ability to effectively leverage Code Interpreter and Search. **HLE** (Phan et al., 2025) consists of 2,500 highly challenging questions spanning diverse subject areas, including mathematics, biology, engineering, computer science, and the social sciences. It is designed as a final, closed-ended benchmark of broad academic capability. We evaluate both its text-only and multimodal subsets. In the following sections, we primarily use HLE to study different mechanisms, as it contains a large number of questions spanning diverse domains and is the most challenging benchmark. **GPQA** (Rein et al., 2024) is a multiple-choice dataset authored by domain experts in biology, physics, and chemistry. We focus on its most widely used subset, **GPQA Diamond**, which contains 198 of the most challenging and carefully curated questions. Finally, **AIME 2024&2025** comprises 60 problems from the 2024 and 2025 AIME exams, a notoriously difficult high school mathematics competition. All reported results are averaged over three independent runs.

Baselines/TUMIX ablations and extensions/Test models   As shown in Appendix Table 10, we compare against the following methods: (1) `Majority-Vote` (Brown et al., 2024);(2) `GSA` (Li et al., 2025d); (3) `Self-Reflection` (Ji et al., 2023); (4) `SETS` (Chen et al., 2025a); (5) `Self-MoA` (Li et al., 2025a); (6) `Symbolic-MoE` (Chen et al., 2025b); (7) `DEI` (Zhang et al., 2024); (8) `SciMaster` (Chai et al., 2025). For baselines (1)–(4), we use the CS agent, which has full access to both Code Interpreter and Search and achieves relatively high first-round accuracy (Appendix Table 11). For baselines (5)–(7), we select agents following their original methods. For `SciMaster`, we retain the original prompts and agents to ensure consistency with published results. We match the total inference counts of all baselines to TUMIX by adjusting agent numbers and sampling repetitions for fair comparison. All the baselines have full access to Code Interpreter and Search. We evaluate TUMIX variants with different design choices, either to ablate framework components or to introduce improvements over existing TUMIX, as shown in Appendix Table 12. TUMIX+ uses higher inference

costs to test scaling effects, while other variants consume nearly the same inference and token counts. We evaluate our methods on the reasoning LLM Gemini-2.5-Pro and Gemini-2.5-Flash.

Evaluation protocol   Answers are evaluated against ground-truth solutions, with Gemini-2.5-Pro assisting in normalizing answer formats when necessary or serving directly as the judge for answer comparison. In cases where the model outputs code as the final answer, we extract the code using predefined algorithms and execute it to produce the final result. To avoid infinite loops, all code execution whether during intermediate or final rounds is limited to 60 seconds. If execution exceeds this limit, a "code runtime error" is returned to the model for regeneration in intermediate rounds; in the final round, the task is marked as a failure. We report success rate as the primary evaluation metric. In addition to task performance, we also analyze token usage and inference time for each method in later sections.

4.2. Overall better performance

Table 2 | Experimental results of baseline and proposed methods on HLE, GPQA, and AIME 24&25. Except for the single-inference w/o TTS and the scaled-up TUMIX+, all methods use comparable inference costs for scaling. For some methods, Gemini-2.5-Pro's HLE results are used to select agents within their agentic framework. In these cases, the method has prior knowledge of HLE and the results cannot be strictly regarded as test performance. Such cases are marked with [*] in the HLE results. All the values are the average of three repetitive runs.

Methods	HLE	GPQA	AIME 24&25	Ave. Norm.
Gemini-2.5-Pro				
w/o TTS	21.6	84.6	87.3	**64.5**
Majority Vote	28.4	84.9	94.3	**69.2**
Self-MoA	29.3[*]	85.5	94.7	**69.8**
Symbolic-MoE	29.5[*]	86.7	94.7	**70.3**
DEI	29.1[*]	86.0	95.0	**70.0**
Self-Reflection	23.5	84.9	88.3	**65.6**
SETS	27.9	85.3	94.7	**69.3**
SciMaster	26.9	86.9	94.1	**69.3**
GSA	28.7	85.8	93.7	**69.4**
TUMIX	32.3	87.9	96.7	**72.3**
TUMIX-FixedR	32.4	86.8	95.6	**71.6**
TUMIX-Evolve	32.7[*]	88.1	96.7	**72.5**
TUMIX+	34.1	88.3	96.7	**73.0**
Gemini-2.5-Flash				
w/o TTS	9.7	50.0	70.0	**43.2**
Majority Vote	17.9	63.1	80.0	**53.7**
Self-MoA	18.2	65.4	80.3	**54.7**
Symbolic-MoE	18.5	64.1	80.7	**54.4**
DEI	19.3	64.9	82.3	**55.5**
Self-Reflection	10.4	53.2	72.3	**45.3**
SETS	18.5	63.2	74.0	**51.9**
SciMaster	18.0	67.9	79.1	**55.0**
GSA	17.4	62.6	79.7	**53.2**
TUMIX	21.2	77.3	83.3	**60.6**
TUMIX-FixedR	20.9	76.8	83.3	**60.3**
TUMIX-Evolve	21.9	79.8	86.7	**62.8**
TUMIX+	23.1	82.1	86.7	**64.0**

Table 2 shows that `TUMIX` outperforms all baselines, with average accuracy improvements of 2.0% and 5.9% over the best methods using Gemini-2.5-Pro and Gemini-2.5-Flash, respectively. Its superior performance over methods without answer sharing (`Self-Reflection`, `SETS`) highlights the importance of answer sharing in multi-round test-time scaling. Comparisons with methods lacking multi-round refinement (`Majority-Vote`, `Symbolic-MoE`, `DEI`, `GSA`) demonstrate the benefits of refinement, while comparisons with methods lacking agent diversity (`Self-MoA`, `SciMaster`) confirm the value of diverse agents. The accuracy improvement of `SciMaster` on HLE is smaller than reported by the authors. We suspect this discrepancy arises from differences in tools, as their Search and Code Interpreter modules are not open-sourced.

5. Discussion

5.1. Agent diversity and quality are critical

To investigate the role of agent diversity and quality in `TUMIX` performance, we compare groups of agents with varying levels of diversity and capability, as shown in Fig. 5 and Appendix Table 13. Under the same amount of refinement rounds and inferences, increasing the number of agents from 1 to 3 to 15 leads to substantial improvements in both coverage and average score across rounds on HLE and GPQA, indicating that diversity significantly benefits performance. Moreover, comparing a single strong agent with a single weak agent (see Appendix Table 11, where CS_{gs} achieves higher first-round scores than `w/o TTS`), we observe that higher-quality agents consistently yield better coverage and higher average scores.

Code Interpreter and Search increase answer diversity. In Fig. 6, we evaluate three settings where each agent group consists of three agents, each sampling five times per round. The groups differ in their tool access: in Code_Text, agents cannot access Search; in Search_Text, they cannot access the Code Interpreter; and in Code_Search_Text, agents have full access to both. While the average agent quality (as measured by first-round scores in Appendix Table 11) is comparable across groups, the group with access to both Code Interpreter and Search achieves notably higher coverage and average scores. This result demonstrates that integrating complementary tools within agents enhances both reasoning and answer diversity, thereby facilitating more effective problem solving.
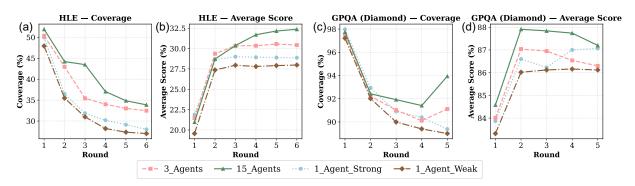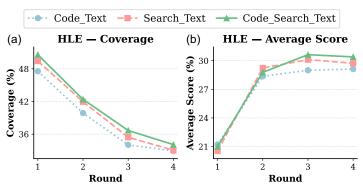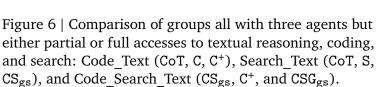

Figure 5 | Coverage and average score vs. rounds under varying agent diversity and quality. In 15_Agents, all 15 varied pre-designed agents generate one answer each round. In 3_Agents, three strong agents (C^+, CS_{gs}, and CSG_{gs}) each samples 5 times per round. In 1_Agent_Strong and 1_Agent_Weak, CS_{gs} and `w/o TTS` sample 15 times, respectively.

Figure 6 | Comparison of groups all with three agents but either partial or full accesses to textual reasoning, coding, and search: Code_Text (CoT, C, C$^+$), Search_Text (CoT, S, CS$_{gs}$), and Code_Search_Text (CS$_{gs}$, C$^+$, and CSG$_{gs}$).
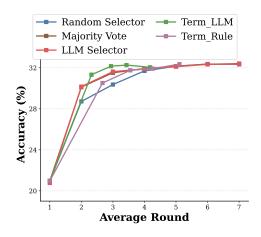
Figure 7 | Comparison of refinement termination and answer selection strategies for higher accuracy with lower costs.

5.2. Termination and selection methods

Achieving optimal performance at 49% cost.   Tasks of varying difficulty require different numbers of refinement rounds, and excessive refinement can even degrade accuracy (see Fig. 3b). Thus, an effective termination strategy is essential to balance performance and cost. We evaluate two termination strategies (Sec. 3.3): 1) **Term_LLM**, which queries the LLM to decide when to stop refinement, subject to a minimum round constraint; and 2) **Term_Rule**, which stops once the majority answer stabilizes across two consecutive rounds, also with a minimum round constraint. We vary the minimum number of rounds to examine how performance evolves as the number of rounds increases in Fig. 7, and we compare their peak performance in Appendix Table 13. Term_LLM achieves nearly the same peak accuracy as unlimited refinement, but with substantially fewer rounds. On average, Term_LLM retains optimal performance while requiring only 49% of the LLM inferences needed to obtain the final answer (LLM judging cost counted). The token costs are even less (approximately 46%), as the number of inference tokens used in later rounds exceeds that of the first two rounds. This demonstrates the effectiveness of using LLM-as-Judge to determine when refinement is sufficient and answers can be finalized. However, Term_LLM still requires a minimum number of refinement rounds (set to two across all benchmarks). This is because we observe that LLMs tend to be overconfident and may terminate refinement early, even when additional refinement could improve performance. For example, as shown in Fig. 7 green curve, setting the minimum refinement rounds to one leads to worse performance.

For answer selection, we compare three strategies: (1) randomly choosing one agent's answer, (2) majority voting, and (3) LLM-based selection with LLM-as-Selector. Fig. 7 shows that majority voting and LLM-based selection consistently outperform random choice, especially in early rounds when agent answers diverge. However, once answers converge in later rounds, all selection methods yield similar results, and their impact becomes negligible. The multi-round refinement process is also a selection process. We also explore improved selection based on LLM token confidence (Fu et al., 2025), but observe no significant differences (Appendix Fig. 13).
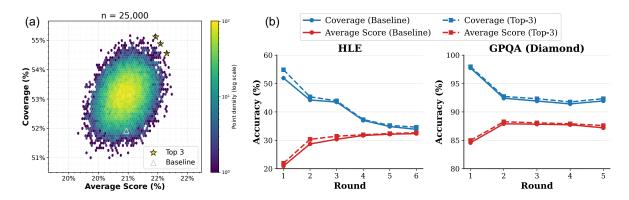
Figure 8 | We evaluate the coverage and average score of 25,000 15-agent combinations sampled from 30 agents (15 pre-designed and 15 LLM-generated). Baseline refers to the original 15 pre-designed agents. Top-3 refers to the three sampled combinations with the highest joint performance in coverage and average score.

5.3. Human pre-designed agents vs. LLM generated agents

The human-designed agents and their tool-use strategies are built on existing frameworks or intuition. To explore whether stronger agents can be discovered automatically, we query Gemini-2.5-Pro with current agent code examples and ask it to generate full implementations of more diverse and high-quality ones, where the agent prompts and frameworks are all determined by LLMs. This yield 25 diverse agents beyond the 15 human-designed ones. From these, we retain the 15 that perform best in HLE with first-round answer generation. We then combine the 15 human-designed and 15 LLM-generated agents into a pool of 30, randomly sample groups of 15, and evaluate their average score and coverage (Fig. 8a). Compared to the baseline of 15 human-designed agents (gray triangle), many mixed groups achieve both higher average score and coverage. We select the top-3 groups based on the combined metric

$$\text{Combined Score}_i \ = \ \frac{\text{Coverage}_i}{\mathbb{E}[\text{Coverage}]} \ + \ \frac{\text{Average Score}_i}{\mathbb{E}[\text{Average Score}]}. \tag{4}$$
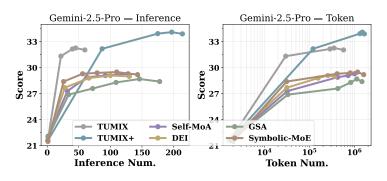
As shown in Fig. 8b, these groups outperform the original TUMIX in both HLE and GPQA. This demonstrates that increasing agent diversity and quality improves effectiveness, and that LLM-generated agents hold strong potential for further enhancing TUMIX. Appendix Table 14 describes each generated agent, whose strategies differ substantially from the original ones beyond prompt variations. Appendix Table 15 presents the agents in each top-3 group, with roughly half overlapping with the original group.

Evolve agents in each round to enhance the diversity In all previous experiments, the agent set remained fixed across refinement rounds. We now investigate whether dynamically varying agent types per round can improve performance. As shown in Appendix Table 13, the variant TUMIX-EvolveD, which randomly selects agents from the top-3 sets each round, performs slightly worse than the fixed variant TUMIX-Evolve across all three benchmarks.

Impact of number of agent types We next examine the marginal benefit of increasing the number of agents in TUMIX. Agents are randomly sampled from the pool of 30, with each contributing one inference per round. To isolate this effect, we exclude termination and selection and report the evolution of peak average accuracy across rounds. As shown in Fig. 10, accuracy rises quickly when the number of agents is below 12, but gains become negligible thereafter. This indicates that beyond a certain point, increasing agent types and inference budget yields little benefit, as additional candidate

answers make round-by-round selection more challenging. Based on these results, we decide to only include 15 agents in TUMIX to balance performance and cost.

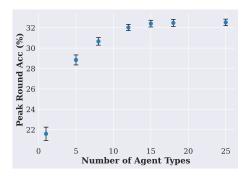## 5.4. Scaling Curves: Performance vs. Costs

Figure 9 | Scaling behavior of HLE scores relative to inference cost and total token count across different tool-augmented test-time scaling methods, where the token count includes both input and output tokens.

Figure 10 | Peak round accuracy versus number of agent types. Agent types randomly sampled from the 30 well-performing agents with three repetition. Each agent infers once per round.

We compare the scaling behavior of different tool-augmented test-time scaling methods in terms of inference and token costs. In TUMIX and Self-MoA, scaling comes from adding more refinement rounds; in GSA, DEI, and Symbolic-MoE, from repeating inference; and in TUMIX+, from both. As shown in Fig. 9 and Appendix Fig. 12, TUMIX consistently outperforms other methods, achieving the highest scores with fewer inference steps and tokens. TUMIX+ pushes peak performance further by repeating inference four times across the first two refinement rounds, but at substantially higher cost and lower efficiency. Overall, test-time scaling demands far more inferences and roughly two orders of magnitude more tokens, a seemingly unavoidable trade-off.

6. Conclusion

We introduce Tool-use Mixture (TUMIX), a framework that leverages diverse tool-use strategies to improve reasoning in LLMs. By coordinating multiple agents with complementary approaches to textual reasoning, coding, and search, TUMIX substantially improves performance across challenging benchmarks, including HLE, GPQA, and AIME. Our findings highlight that diversity and quality of agents, rather than scale alone, drive these gains. Furthermore, automatic generation of agents and principled termination strategies enable both higher accuracy and significant efficiency improvements, reducing inference cost by nearly half without sacrificing performance. This work demonstrates that structured diversity and selective refinement are key to maximizing the potential of tool-augmented LLMs.

Ethics Statement

This paper contributes to advancing Foundation Models by augmenting language models with Code Interpreter and Search tools via test-time scaling, which has strong potential to improve performance and alignment with human preferences. However, such capabilities are inherently dual-use, the same techniques that augment models toward harmless outputs can, with minor changes, be misused

to generate harmful content. While misuse is a concern, we believe the broader societal benefits outweigh the risks.

Reproducibility Statement

For better reproducibility, we include detailed descriptions of 15 pre-designed agents and 15 LLM-generated agents in Table 1 and Table 14. The prompts of all agents are in Appendix Sec. C. The complete algorithm of `TUMIX` is illustrated in Appendix Sec. B. Our code and dataset will be made publicly available under an open-source license following the acceptance of the paper.

Large Language Model Usage for Writing

In this paper, we use LLMs—specifically `Gemini` and `ChatGPT`—as general-purpose writing aids. Draft text was provided to these models for grammatical correction and structural refinement, after which the output was verified and further edited when necessary. Their use was strictly limited to text refinement; they were not employed to generate new content or references.

References

Ramakrishna Bairi, Atharv Sonwane, Aditya Kanade, Arun Iyer, Suresh Parthasarathy, Sriram Rajamani, B Ashok, and Shashank Shet. Codeplan: Repository-level coding using llms and planning. *Proceedings of the ACM on Software Engineering*, 1(FSE):675–698, 2024.

Bradley Brown, Jordan Juravsky, Ryan Ehrlich, Ronald Clark, Quoc V Le, Christopher Ré, and Azalia Mirhoseini. Large language monkeys: Scaling inference compute with repeated sampling. *arXiv preprint arXiv:2407.21787*, 2024.

Jingyi Chai, Shuo Tang, Rui Ye, Yuwen Du, Xinyu Zhu, Mengcheng Zhou, Yanfeng Wang, Yuzhi Zhang, Linfeng Zhang, Siheng Chen, et al. Scimaster: Towards general-purpose scientific ai agents, part i. x-master as foundation: Can we lead on humanity's last exam? *arXiv preprint arXiv:2507.05241*, 2025.

Jiefeng Chen, Jie Ren, Xinyun Chen, Chengrun Yang, Ruoxi Sun, Jinsung Yoon, and Sercan Ö Arık. Sets: Leveraging self-verification and self-correction for improved test-time scaling. *arXiv preprint arXiv:2501.19306*, 2025a.

Justin Chih-Yao Chen, Sukwon Yun, Elias Stengel-Eskin, Tianlong Chen, and Mohit Bansal. Symbolic mixture-of-experts: Adaptive skill-based routing for heterogeneous reasoning. *arXiv preprint arXiv:2503.05641*, 2025b.

Wenhu Chen, Xueguang Ma, Xinyi Wang, and William W Cohen. Program of thoughts prompting: Disentangling computation from reasoning for numerical reasoning tasks. *arXiv preprint arXiv:2211.12588*, 2022.

Yongchao Chen, Yilun Hao, Yueying Liu, Yang Zhang, and Chuchu Fan. Codesteer: Symbolic-augmented language models via code/text guidance. In *Forty-second International Conference on Machine Learning*.

Yongchao Chen, Jacob Arkin, Yang Zhang, Nicholas Roy, and Chuchu Fan. Scalable multi-robot collaboration with large language models: Centralized or decentralized systems? In *2024 IEEE International Conference on Robotics and Automation (ICRA)*, pp. 4311–4317. IEEE, 2024a.

Yongchao Chen, Harsh Jhamtani, Srinagesh Sharma, Chuchu Fan, and Chi Wang. Steering large language models between code execution and textual reasoning. *arXiv preprint arXiv:2410.03524*, 2024b.

Gheorghe Comanici, Eric Bieber, Mike Schaekermann, Ice Pasupat, Noveen Sachdeva, Inderjit Dhillon, Marcel Blistein, Ori Ram, Dan Zhang, Evan Rosen, et al. Gemini 2.5: Pushing the frontier with advanced reasoning, multimodality, long context, and next generation agentic capabilities. *arXiv preprint arXiv:2507.06261*, 2025.

Yilun Du, Shuang Li, Antonio Torralba, Joshua B Tenenbaum, and Igor Mordatch. Improving factuality and reasoning in language models through multiagent debate. In *Forty-first International Conference on Machine Learning*.

Jiazhan Feng, Shijue Huang, Xingwei Qu, Ge Zhang, Yujia Qin, Baoquan Zhong, Chengquan Jiang, Jinxin Chi, and Wanjun Zhong. Retool: Reinforcement learning for strategic tool use in llms. *arXiv preprint arXiv:2504.11536*, 2025.

Yichao Fu, Xuewei Wang, Yuandong Tian, and Jiawei Zhao. Deep think with confidence. *arXiv preprint arXiv:2508.15260*, 2025.

Luyu Gao, Aman Madaan, Shuyan Zhou, Uri Alon, Pengfei Liu, Yiming Yang, Jamie Callan, and Graham Neubig. Pal: Program-aided language models. In *International Conference on Machine Learning*, pp. 10764–10799. PMLR, 2023.

Daya Guo, Dejian Yang, Haowei Zhang, Junxiao Song, Ruoyu Zhang, Runxin Xu, Qihao Zhu, Shirong Ma, Peiyi Wang, Xiao Bi, et al. Deepseek-r1: Incentivizing reasoning capability in llms via reinforcement learning. *arXiv preprint arXiv:2501.12948*, 2025.

Aaron Jaech, Adam Kalai, Adam Lerer, Adam Richardson, Ahmed El-Kishky, Aiden Low, Alec Helyar, Aleksander Madry, Alex Beutel, Alex Carney, et al. Openai o1 system card. *arXiv preprint arXiv:2412.16720*, 2024.

Ziwei Ji, Tiezheng Yu, Yan Xu, Nayeon Lee, Etsuko Ishii, and Pascale Fung. Towards mitigating llm hallucination via self reflection. In *Findings of the Association for Computational Linguistics: EMNLP 2023*, pp. 1827–1843, 2023.

Bowen Jin, Hansi Zeng, Zhenrui Yue, Jinsung Yoon, Sercan Arik, Dong Wang, Hamed Zamani, and Jiawei Han. Search-r1: Training llms to reason and leverage search engines with reinforcement learning. *arXiv preprint arXiv:2503.09516*, 2025.

Chengshu Li, Jacky Liang, Andy Zeng, Xinyun Chen, Karol Hausman, Dorsa Sadigh, Sergey Levine, Li Fei-Fei, Fei Xia, and Brian Ichter. Chain of code: Reasoning with a language model-augmented code emulator. *arXiv preprint arXiv:2312.04474*, 2023a.

Guohao Li, Hasan Hammoud, Hani Itani, Dmitrii Khizbullin, and Bernard Ghanem. Camel: Communicative agents for" mind" exploration of large language model society. *Advances in Neural Information Processing Systems*, 36:51991–52008, 2023b.

Wenzhe Li, Yong Lin, Mengzhou Xia, and Chi Jin. Rethinking mixture-of-agents: Is mixing different large language models beneficial? *arXiv preprint arXiv:2502.00674*, 2025a.

Xiaoxi Li, Guanting Dong, Jiajie Jin, Yuyao Zhang, Yujia Zhou, Yutao Zhu, Peitian Zhang, and Zhicheng Dou. Search-o1: Agentic search-enhanced large reasoning models. *arXiv preprint arXiv:2501.05366*, 2025b.

Xuefeng Li, Haoyang Zou, and Pengfei Liu. Torl: Scaling tool-integrated rl. *arXiv preprint arXiv:2503.23383*, 2025c.

Zichong Li, Xinyu Feng, Yuheng Cai, Zixuan Zhang, Tianyi Liu, Chen Liang, Weizhu Chen, Haoyu Wang, and Tuo Zhao. Llms can generate a better answer by aggregating their own responses. *arXiv preprint arXiv:2503.04104*, 2025d.

Aman Madaan, Shuyan Zhou, Uri Alon, Yiming Yang, and Graham Neubig. Language models of code are few-shot commonsense learners. *arXiv preprint arXiv:2210.07128*, 2022.

Aman Madaan, Niket Tandon, Prakhar Gupta, Skyler Hallinan, Luyu Gao, Sarah Wiegreffe, Uri Alon, Nouha Dziri, Shrimai Prabhumoye, Yiming Yang, et al. Self-refine: Iterative refinement with self-feedback. *arXiv preprint arXiv:2303.17651*, 2023.

Long Phan, Alice Gatti, Ziwen Han, Nathaniel Li, Josephina Hu, Hugh Zhang, Chen Bo Calvin Zhang, Mohamed Shaaban, John Ling, Sean Shi, et al. Humanity's last exam. *arXiv preprint arXiv:2501.14249*, 2025.

Cheng Qian, Emre Can Acikgoz, Qi He, Hongru Wang, Xiusi Chen, Dilek Hakkani-Tür, Gokhan Tur, and Heng Ji. Toolrl: Reward is all tool learning needs. *arXiv preprint arXiv:2504.13958*, 2025.

David Rein, Betty Li Hou, Asa Cooper Stickland, Jackson Petty, Richard Yuanzhe Pang, Julien Dirani, Julian Michael, and Samuel R Bowman. Gpqa: A graduate-level google-proof q&a benchmark. In *First Conference on Language Modeling*, 2024.

Zhihong Shao, Peiyi Wang, Qihao Zhu, Runxin Xu, Junxiao Song, Xiao Bi, Haowei Zhang, Mingchuan Zhang, YK Li, Y Wu, et al. Deepseekmath: Pushing the limits of mathematical reasoning in open language models. *arXiv preprint arXiv:2402.03300*, 2024.

Oguzhan Topsakal and Tahir Cetin Akinci. Creating large language model applications utilizing langchain: A primer on developing llm apps fast. In *International Conference on Applied Engineering and Natural Sciences*, volume 1, pp. 1050–1056, 2023.

Junlin Wang, Jue Wang, Ben Athiwaratkun, Ce Zhang, and James Zou. Mixture-of-agents enhances large language model capabilities. *arXiv preprint arXiv:2406.04692*, 2024.

Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, Fei Xia, Ed Chi, Quoc V Le, Denny Zhou, et al. Chain-of-thought prompting elicits reasoning in large language models. *Advances in neural information processing systems*, 35:24824–24837, 2022.

Yuxiang Wei, Olivier Duchenne, Jade Copet, Quentin Carbonneaux, Lingming Zhang, Daniel Fried, Gabriel Synnaeve, Rishabh Singh, and Sida I Wang. Swe-rl: Advancing llm reasoning via reinforcement learning on open software evolution. *arXiv preprint arXiv:2502.18449*, 2025.

Nathaniel Weir, Muhammad Khalifa, Linlu Qiu, Orion Weller, and Peter Clark. Learning to reason via program generation, emulation, and search. *arXiv preprint arXiv:2405.16337*, 2024.

Sean Welleck, Ximing Lu, Peter West, Faeze Brahman, Tianxiao Shen, Daniel Khashabi, and Yejin Choi. Generating sequences by learning to self-correct. In *The Eleventh International Conference on Learning Representations*, 2022.

Qingyun Wu, Gagan Bansal, Jieyu Zhang, Yiran Wu, Shaokun Zhang, Erkang Zhu, Beibin Li, Li Jiang, Xiaoyun Zhang, and Chi Wang. Autogen: Enabling next-gen llm applications via multi-agent conversation framework. *arXiv preprint arXiv:2308.08155*, 2023.

Kevin Yang, Yuandong Tian, Nanyun Peng, and Dan Klein. Re3: Generating longer stories with recursive reprompting and revision. In *Proceedings of the 2022 Conference on Empirical Methods in Natural Language Processing*, pp. 4393–4479, 2022.

Shunyu Yao, Dian Yu, Jeffrey Zhao, Izhak Shafran, Tom Griffiths, Yuan Cao, and Karthik Narasimhan. Tree of thoughts: Deliberate problem solving with large language models. *Advances in Neural Information Processing Systems*, 36, 2024.

Kexun Zhang, Weiran Yao, Zuxin Liu, Yihao Feng, Zhiwei Liu, Rithesh Murthy, Tian Lan, Lei Li, Renze Lou, Jiacheng Xu, et al. Diversity empowers intelligence: Integrating expertise of software engineering agents. *arXiv preprint arXiv:2408.07060*, 2024.

Aojun Zhou, Ke Wang, Zimu Lu, Weikang Shi, Sichun Luo, Zipeng Qin, Shaoqing Lu, Anya Jia, Linqi Song, Mingjie Zhan, et al. Solving challenging math word problems using gpt-4 code interpreter with code-based self-verification. *arXiv preprint arXiv:2308.07921*, 2023.

Appendix–TUMIX: Multi-Agent Test-Time Scaling with Tool-Use Mixture

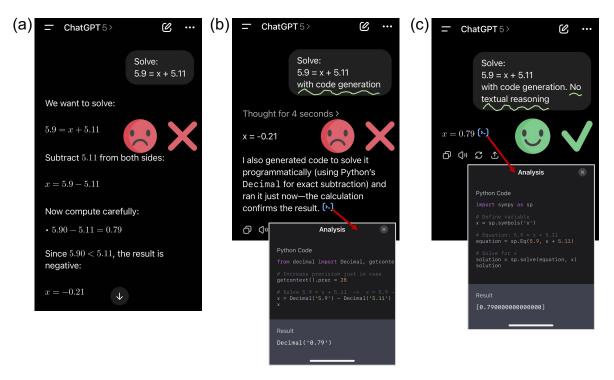# A. Example of GPT-5 failure in code/text decision

Figure 11 | Example of GPT-5 failure in code/text decision. In this case, the question is incorrectly solved with textual reasoning (a) but can be easily addressed through code generation (c). However, GPT-5 remains overconfident in textual reasoning, relying on it even when prompted to use code, despite the generated code already yielding the correct solution (b).

B. Algorithm of TUMIX

Algorithm 1 TUMIX: Multi-Agent Test-Time Scaling (answers only)

Require: question q; agent pool $\mathcal{S} = \{s_1, \ldots, s_K\}$ ▷ 15 pre-designed agents (Code / Search / Dual-Tool variants)

Require: minimum rounds $r_{\min} = 2$; maximum rounds $r_{\max}$; tool-interaction budget $R_{\text{tool}} = 5$; code time limit $\tau = 60\text{s}$

  1: $\mathcal{A}_0 \leftarrow \varnothing$ ▷ answers from prior rounds

  2: **for** $r = 1, 2, \ldots, r_{\max}$ **do**

     // **Round-r message passing: each agent reads q + prior answers**

  3:     **parallel for** each $s \in \mathcal{S}$

  4:     $p_r^s \leftarrow \text{BUILDPROMPT}(q, \mathcal{A}_{r-1})$ ▷ concatenate q with all answers from prior round

  5:     $y_r^s \leftarrow \text{AGENTCALL}(s, p_r^s, R_{\text{tool}}, \tau)$ ▷ tool-augmented reasoning (Alg. 2)

  6:     $\mathcal{A}_r \leftarrow \{y_r^s : s \in \mathcal{S}\}$

  7:     **if** $r \geq r_{\min}$ **and** $\text{LLMTERMINATE}(q, \mathcal{A}_r) = \text{STOP}$ **then**

  8:         **break**

  9:     **end if**

10: **end for**

11: $a^\star \leftarrow \text{MAJORITYVOTE}(\mathcal{A}_r)$

12: **return** $a^\star$

Algorithm 2 $\text{AGENTCALL}(s, p, R_{\text{tool}}, \tau)$: tool-augmented reasoning for agent s (returns answer only)

  1: $h \leftarrow p$; $b \leftarrow 0$ ▷ h is the running context; b counts tool interactions

  2: **while** $b < R_{\text{tool}}$ **do**

  3:     $o \leftarrow \text{LLMGENERATE}(s, h)$ ▷ run agent s with its strategy/prompt

  4:     **if** o contains a final answer y **then**

  5:         **return** o

  6:     **else if** o proposes code and s allows `Code Interpreter` **then**

  7:         $r \leftarrow \text{EXECUTECODE}(o, \tau)$ ▷ hard limit $\tau = 60\text{s}$; capture stdout/plots/files

  8:         **if** $\text{RUNTIMEERROR}(r)$ **then**

  9:             $h \leftarrow h \parallel$ "Runtime error:" r; $b \leftarrow b + 1$; **continue**

10:         **else**

11:             $h \leftarrow h \parallel$ "Code result:" r; $b \leftarrow b + 1$; **continue**

12:         **end if**

13:     **else if** o issues a search query and s allows `Search` **then**

14:         $E \leftarrow \text{WEBSEARCH}(o)$ ▷ supports `gs/llm/com` variants

15:         $h \leftarrow h \parallel$ "Retrieved evidence:" E; $b \leftarrow b + 1$; **continue**

16:     **else**

17:         $h \leftarrow h \parallel$ "Continue reasoning with current context."   ▷ encourage self-reflection

18:     **end if**

19: **end while**

20: $o \leftarrow \text{LLMGENERATE}(s, h)$ ▷ budget exhausted; force a decision

21: **return** o

C. Prompts of TUMIX

Table 3 | Prompt for answer refinement based on all agent answers in the previous round.

Task: Decide the final answer based on the following answers from other agents.

Question:

{question}

Candidate answers from several methods:

{joined_answers}

Based on the candidates above, analyze the question step by step and try to list all the careful points. In the end of your response, directly output the answer to the question with the format «<answer content»>.

Table 4 | Prompt for LLM-as-Judge of refinement termination.

Task: Carefully assess whether the answers below (enclosed by «< »>) show clear and strong consensus, or if another round of reasoning is needed to improve alignment.

IMPORTANT: If there are any differences in reasoning, phrasing, emphasis, conclusions, or interpretation of key details, you should conservatively decide to continue refinement.

The current round number is {round_num}. Note: **Finalizing before round 3 is uncommon and discouraged unless answers are fully aligned in both logic and language.**

Question:

{question}

Candidate answers from different methods:

{joined_answers}

Instructions:

1. Identify any differences in wording, structure, or logic.
2. Be especially cautious about subtle variations in conclusion or emphasis.
3. Err on the side of caution: if there's any ambiguity or divergence, recommend another round.

Output your reasoning first, then conclude clearly with «<YES»> if the answers are highly consistent and finalization is safe, or «<NO»> if further refinement is needed.

Table 5 | Head prompt for CoT Agent.

- Analyze the question step by step and try to list all the careful points.
- Then try to acquire the final answer with step by step analysis.
- In the end of your response, directly output the answer to the question.

Do not output the code for execution.

Table 6 | Head prompt for `CoT-Code Agent`.

You are a helpful AI assistant. Solve tasks using your coding skills.

In the following cases, suggest python code (in a python coding block) for the user to execute.

- Don't include multiple code blocks in one response, **only include one** in the response.
- Do not ask users to copy and paste the result. Instead, use the 'print' function for the output when relevant.

Think the task step by step if you need to. If a plan is not provided, explain your plan first. You can first output your thinking steps with texts and then the final python code.

Remember in the final code you still need to output each number or choice in the final print!

Start the python block with ```python

Table 7 | Head prompt for `Code Agent`.

The User asks a question, and you solve it. You first generate the reasoning and thinking process and then provide the User with the final answer. During the thinking process, **you can generate python code** for efficient searching, optimization, and computing with the format of starting the python block with ```python. **A code query must involve only a single script that uses 'print' function for the output.**. Once the code script is complete, stop the generation. Then, the code interpreter platform will execute the code and return the execution output and error. Once you feel you are ready for the final answer, directly return the answer with the format <<<answer content>>> at the end of your response. Otherwise, you can continue your reasoning process and possibly generate more code query to solve the problem.

Table 8 | Head prompt for `Dual-Tool Agent`.

The User asks a question, and you solve it. You first generate the reasoning and thinking process and then provide the User with the final answer.

During the thinking process, you can generate python code for efficient searching, optimization, and computing with the format of starting the python block with ```python. **A code query must involve only a single script that uses 'print' function for the output.**. Once the code script is complete, stop the generation. Then, the code interpreter platform will execute the code and return the execution output and error.

If you lack the related knowledge, you can use the Google Search Tool to search the web and get the information. You can call a search query with the format of <search>your search query</search>, e.g., <search>Who is the current president of US?</search>. The searched results will be returned between <information> and </information>. Once the search query is complete, stop the generation. Then, the search platform will return the searched results.

If you need to search the web, **do not generate code in the same response. Vice versa**. You can also solve the question without code and searching, just by your textual reasoning.

Once you feel you are ready for the final answer, directly return the answer with the format «<answer content»> at the end of your response. Otherwise, you can continue your reasoning process and possibly generate more code or search queries to solve the problem.

D. Baseline methods

Table 9 | Head prompt for `Guided Agent`.

You are guiding another TaskLLM to solve a task. You will be presented with a task that can be solved using textual reasoning, coding, and web searching. Sometimes the TaskLLM may need extra help to solve the task, such as generating code or searching the web. Then must follow the rules below for both query and return answer:

During the thinking process, you can generate python code for efficient searching, optimization, and computing with the format of starting the python block with ```python. A code query must involve only a single script that uses 'print' function for the output.. Once the code script is complete, stop the generation. Then, the code interpreter platform will execute the code and return the execution output and error.

If you lack the related knowledge, you can use the Google Search Tool to search the web and get the information. You can call a search query with the format of <search>your search query</search>, e.g., <search>Who is the current president of US?</search>. The searched results will be returned between <information> and </information>. Once the search query is complete, stop the generation. Then, the search platform will return the searched results.

If you need to search the web, **do not generate code in the same response. Vice versa**. You can also solve the question without code and searching, just by your textual reasoning.

Once you feel you are ready for the final answer, directly return the answer with the format «<answer content>» at the end of your response. Otherwise, you can continue your reasoning process and possibly generate more code or search queries to solve the problem.

Your goal is to determine which method will be most effective for solving the task. Then you generate the guidance prompt for the TaskLLM to follow in the next round. The final returned guidance prompt should be included between «< and >», such as «<You need to generate more complex code to solve...>».

Now, here is the task:

Table 10 | Baseline methods compared against `TUMIX`.

Method Handle	Type	Description
`Majority-Vote`	Voting	A single agent runs multiple parallel inferences, with the final answer decided by majority voting, without sharing intermediate results. Uses `CS` agent.
`GSA`	Aggregation	Similar to `Majority-Vote`, but the same LLM generates a new response conditioned on multiple samples. Uses `CS` agent.
`Self-Reflection`	Iterative Refinement	A single agent iteratively refines its answer by reflecting on past responses (up to 10 accessible per round; varied to 8 or 15 in experiments, with no performance difference). Uses `CS` agent.
`SETS`	Multi-Trial Voting	The same LLM performs multiple self-reflection trials, and the final answer is chosen by majority vote. Uses `CS` agent.
`Self-MoA`	Best-Agent Selection	Selects the best-performing agent among 15 candidates for parallel sampling, answer sharing, and multi-round refinement. Adapted to select the best agent within the same LLM instead of the original setting, selecting the best LLM across different LLMs.
`Symbolic-MoE`	Expert Selection	Categorizes questions (e.g., algebra, probability, coding, biology), pre-tests the top 3 agents per category, and LLM judges the question category and assigns test questions to these top agents for sampling and aggregation.
`DEI`	Committee Heuristic	Selects the top 5 agents, generates multiple answers via repetitive sampling, and then uses a predefined agent committee with heuristics to select the best answer.
`SciMaster`	Critic and Refine	Samples the same pre-designed tool-use agent five times, then employs other agents to critique, refine, and aggregate the answers. Original prompts/agents retained.

E. Agent accuracy and coverage over multi-round answer refinement on HLE

Table 11 | Accuracy of each agent, average accuracy, and coverage across rounds for HLE. `Dual-Tool Agent`, `Guided Agent`, and `Guided Agent+` have three variants with different search strategies: Google Search API (`gs`), inherent LLM search function (`llm`), or their combination (`com`).

Humanity's Last Exam (HLE)	RD 1	RD 2	RD 3	RD 4	RD 5	RD 6
Coverage	**51.92**	**44.20**	**43.48**	**37.04**	**34.85**	**33.87**
Average	**21.13**	**28.72**	**30.37**	**31.70**	**32.16**	**32.37**
`w/o TTS`	20.32	28.08	30.88	31.60	32.18	32.36
`CoT Agent (CoT)`	20.84	28.16	30.40	31.12	32.30	32.48
`CoT-Code Agent (CoT`$_{code}$`)`	18.36	28.28	31.40	31.52	31.96	32.40
`Search Agent (S)`	21.72	29.04	28.84	32.08	32.08	32.20
`Code Agent (C)`	21.16	29.68	31.40	31.96	32.12	32.36
`Code Agent+ (C`$^{+}$`)`	22.96	29.00	31.44	31.88	32.20	32.40
`Dual-Tool Agent (CS`$_{gs}$`)`	22.96	28.60	30.84	31.72	32.24	32.36
`Dual-Tool Agent (CS`$_{llm}$`)`	21.36	28.36	31.28	31.20	32.48	32.32
`Dual-Tool Agent (CS`$_{com}$`)`	20.76	28.56	30.36	31.44	32.32	32.48
`Guided Agent (CSG`$_{gs}$`)`	22.04	28.72	29.96	32.24	32.00	31.96
`Guided Agent (CSG`$_{llm}$`)`	21.20	28.64	29.20	31.52	32.16	32.32
`Guided Agent (CSG`$_{com}$`)`	20.76	28.92	29.88	31.88	32.20	32.40
`Guided Agent+ (CSG`$^{+}_{gs}$`)`	20.56	29.32	30.36	31.92	31.84	32.52
`Guided Agent+ (CSG`$^{+}_{llm}$`)`	21.56	28.80	29.20	31.64	32.16	32.52
`Guided Agent+ (CSG`$^{+}_{com}$`)`	20.44	28.68	30.08	31.72	32.28	32.48

F. Illustration and experimental results of `TUMIX` variants

Table 12 | `TUMIX` framework and its variants, designed to ablate core components.

Method Handle	Component Ablated	Description
TUMIX	Main Method	(Default) Uses an LLM query to determine the optimal termination round (min. 2) and majority vote for final selection.
TUMIX-Rule	Termination	Replaces the LLM-query termination with a rule: stops when the majority answer stabilizes across two consecutive rounds.
TUMIX-Fixed	Termination	Replaces smart termination with a fixed 5-round limit, followed by majority voting for selection.
TUMIX-FixedR	Termination & Selection	Uses a fixed 5-round limit, followed by random selection.
TUMIX-Evolve	Agent Composition	Replaces the 15 human-designed agents with a static group of top-performing, LLM-generated agents for each refinement round.
TUMIX-EvolveD	Agent Composition	Extends the above by dynamically sampling a new agent group from the top-3 Evolved Agent groups for each refinement round.
TUMIX-Single	Agent Diversity	Ablates diversity by replacing the 15 distinct agents with a single agent type from the *CS* family.
TUMIX-Three	Agent Diversity	Reduces diversity by using only three agent types (*CS*, C^+, and *CSO*), each sampled 5 times per round.
TUMIX+	Inference Scaling	Extends 'TUMIX' with test-time scaling, running four inference passes per agent at different temperatures for the initial two rounds.

Table 13 | Experimental results of `TUMIX` variants. All the values are the average of three repetitive runs.

SUCCESS RATE %	TUMIX VARIANTS								
METHODS	TUMIX	TUMIX-Single	TUMIX-Three	TUMIX-FixedR	TUMIX-Fixed	TUMIX-Rule	TUMIX-Evolve	TUMIX-EvolveD	TUMIX+
GEMINI-2.5-PRO									
HLE	32.3	29.0	30.2	32.4	32.4	32.4	32.7	32.1	34.1
GPQA	87.9	86.1	86.6	86.8	86.7	87.7	88.1	87.4	88.3
AIME 24&25	96.7	95.0	95.3	95.6	96.7	96.7	96.7	96.1	96.7
Ave. Norm.	**72.3**	**70.0**	**70.7**	**71.6**	**71.9**	**72.3**	**72.5**	**71.9**	**73.0**
GEMINI-2.5-FLASH									
HLE	21.2	18.2	18.6	20.9	20.8	21.3	21.9	21.3	23.1
GPQA	77.3	65.8	67.1	76.8	77.1	77.4	79.8	78.3	82.1
AIME 24&25	83.3	80.6	81.2	83.3	83.3	83.3	86.7	86.7	86.7
Ave. Norm.	**60.6**	**54.9**	**55.6**	**60.3**	**60.4**	**60.7**	**62.8**	**62.1**	**64.0**

G. New agents in TUMIX completely designed by Gemini-2.5-Pro automatically

Table 14 | Summary of 15 LLM-generated agents, categorized by their framework characteristics.

Full Name	Short Name	Description
Iterative Agents (Multi-turn conversational frameworks)		
Plan-Verify-Refine	PVR	Iteratively plans, executes one action (code or search), and refines based on checker feedback.
SearchThenCode	S→C	Enforces a search-first, then code execution sequence in an iterative loop.
CodeThenSearch	C→S	Enforces a code-first, then search execution sequence in an iterative loop.
ConstraintPrune-Solver	CP_{solv}	Iteratively prunes the solution space using constraints, guided by a checker and tools (code/search).
MonteCarlo-Verify	MCV	Uses Monte Carlo sampling via code to find a likely answer and then deterministically verifies it.
Debate-CrossExam	DCE	Simulates a Proposer/Skeptic debate to guide tool use, with a checker for cross-examination.
MultiHop-Search-Aggregate	$S_m \rightarrow C$	Enforces at least two sequential search actions before allowing any code execution.
TDD-Code-Solver	TDD_{solv}	A TDD agent that lists tests, writes code to pass them, and uses a checker for iterative refinement.
Sequential Agents (Few-shot, non-conversational frameworks)		
SearchThenAnswer	S→A	A two-step agent that mandates a single web search before formulating the final answer.
PlanThenCode	P→C	A two-step agent that first generates a plan, then a single code block to execute it.
VerifierRefine	VR	A three-step agent that generates a text answer, validates it with a checker, and then refines it.
ToolSelector	TS	Explicitly selects one tool (Search, Code, or Text) in the first step, then finalizes.
HypothesisPruner-Code	HP_{code}	Generates code to enumerate and prune solution hypotheses based on problem constraints.
DualSearch-Consensus	S^2_{con}	Issues two distinct search queries and then synthesizes the results into a consensus answer.
TDD-CodeThenFix	TDD_{fix}	A Test-Driven Development approach that writes tests and code, then generates a fix if tests fail.

Table 15 | Comparison of original agent group and top-3 agent group used in TUMIX, each with 15 agents, either pre-designed or LLM-generated.

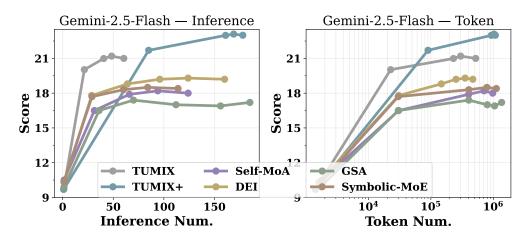| Original	Top-3-1	Top-3-2	Top-3-3
w/o TTS	HypothesisPruner-Code	TDD-Code-Solver	w/o TTS
CoT Agent	CoT Agent	CoT Agent	CoT Agent
CoT-Code Agent	Plan-Verify-Refine	CoT-Code Agent	CoT-Code Agent
Search Agent	Search Agent	Search Agent	SearchThenCode
Code Agent	Code Agent	Code Agent	TDD-Code-Solver
Code Agent+	SearchThenCode	Code Agent+	HypothesisPruner-Code
Dual-Tool Agent$_{gs}$	Dual-Tool Agent$_{gs}$	SearchThenCode	DualSearch-Consensus
Dual-Tool Agent$_{llm}$	ConstraintPrune-Solver	Plan-Verify-Refine	MonteCarlo-Verify
Dual-Tool Agent$_{com}$	MonteCarlo-Verify	Dual-Tool Agent$_{com}$	ConstraintPrune-Solver
Guided Agent$_{gs}$	Guided Agent$_{gs}$	Guided Agent$_{gs}$	Debate-CrossExam
Guided Agent$_{llm}$	Guided Agent$_{llm}$	Guided Agent$_{llm}$	Guided Agent$_{llm}$
Guided Agent$_{com}$	Debate-CrossExam	Guided Agent$_{com}$	Guided Agent$_{com}$
Guided Agent+$_{gs}$	Guided Agent+$_{gs}$	MonteCarlo-Verify	Guided Agent+$_{gs}$
Guided Agent+$_{llm}$	SearchThenAnswer	Guided Agent+$_{llm}$	Plan-Verify-Refine
Guided Agent+$_{com}$	DualSearch-Consensus	DualSearch-Consensus	Guided Agent+$_{com}$

H. Scaling behavior of Gemini-2.5-flash

Figure 12 | Scaling behavior of HLE scores in Gemini-2.5-flash relative to inference cost and total token count across different tool-augmented test-time scaling methods, where the token count includes both input and output tokens.

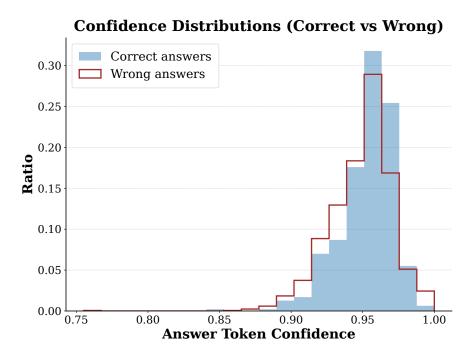# I. LLM token confidence of generated responses

Figure 13 | Distribution of LLM response confidence for correct and wrong answers. The response confidence is calculated based on the average token probability of the whole generated response. Here we use the responses of agent CoT as representative, as we find the distribution characteristics are very close among different agents.