FlowReasoner: Reinforcing Query-Level Meta-Agents

Anonymous authors
Paper under double-blind review

Abstract

This paper proposes a query-level meta-agent named FlowReasoner to automate the design of query-level multi-agent systems, i.e., *one system per user query*. Our core idea is to incentivize a reasoning-based meta-agent via external execution feedback. Concretely, by distilling DeepSeek R1, we first endow the basic reasoning ability regarding the generation of multi-agent systems to FlowReasoner. Then, we further enhance it via reinforcement learning (RL) with external execution feedback. A multi-purpose reward is designed to guide the RL training from aspects of performance, complexity, and efficiency. In this manner, FlowReasoner is enabled to generate a personalized multi-agent system for each user query via deliberative reasoning. Experiments on both engineering and competition code benchmarks demonstrate the superiority of FlowReasoner. Remarkably, it surpasses o1-mini by **10.52**% accuracy across three benchmarks. All the code is included in the Supplemental Material.

1 Introduction

Large language models (LLMs) (Achiam et al., 2023; Reid et al., 2024; Team, 2024a; Yang et al., 2024; Liu et al., 2024) have exhibited remarkable power in various meaningful yet challenging domains, like chatbots (OpenAI, 2022), code (CognitionAI, 2024), math (OpenAI, 2024), robotics (Kim et al., 2024), etc. LLM-based multi-agent systems (Hong et al., 2023; Wu et al., 2023; Li et al., 2023), which are characterized by planning, reasoning, tool use, and memory, become the foundation of these LLM-driven applications.[1] While effective, most of them are manually designed, increasing human resource costs and limiting scalability.

To mitigate this challenge, early automatic methods are proposed to optimize the prompts (Yuksekgonul et al., 2024; Khattab et al., 2024; Zhou et al., 2024a; Yang et al., 2023) or hyper-parameters (Saad-Falcon et al., 2024). But they still rely on the fixed workflow of the multi-agent system, which requires human effort to manually design workflows for each new scenario. From this motivation, various graph-based methods (Zhuge et al., 2024; Liu et al., 2023; Zhang et al., 2024a; Feng et al., 2025; He et al., 2025d;e) formulate the workflows as graphs or networks and automate the workflow designs. However, the structural complexity of graphs limits their scalability (Hu et al., 2024). To overcome this limitation, state-of-the-art methods represent the multi-agent systems as programming codes (Hu et al., 2024) and prompt a performant LLM, e.g., GPT-4o, as a *meta-agent* to optimize workflows via complex search algorithms on carefully designed search sets (Zhang et al., 2024b; Shang et al., 2024; Zhang et al., 2025).

These previous methods focus on **task-level meta-agents**, generating merely a single **task-specific multi-agent system** that applies to one kind of task, e.g., *code generation task*, as in Figure 1 (a). However, for individual user queries, these one-size-fits-all systems lack the capability for automatic adaptation. To enhance the adaptability of multi-agent systems for individual user queries, this paper aims to design a **query-level meta-agent** to generate a **query-specific multi-agent system** for each user query, e.g., *build a 2048 game*, as shown in Figure 1 (b).

We first identify that the success of task-level meta-agents largely depends on carefully designed search sets, as they rely on complex search algorithms. However, such search sets are unavailable in the setting of query-specific multi-agent systems. To address this issue, instead of relying on search algorithms, we

[1]This paper defines a *multi-agent system* as a system consisting of multiple agents operating under a *workflow*.

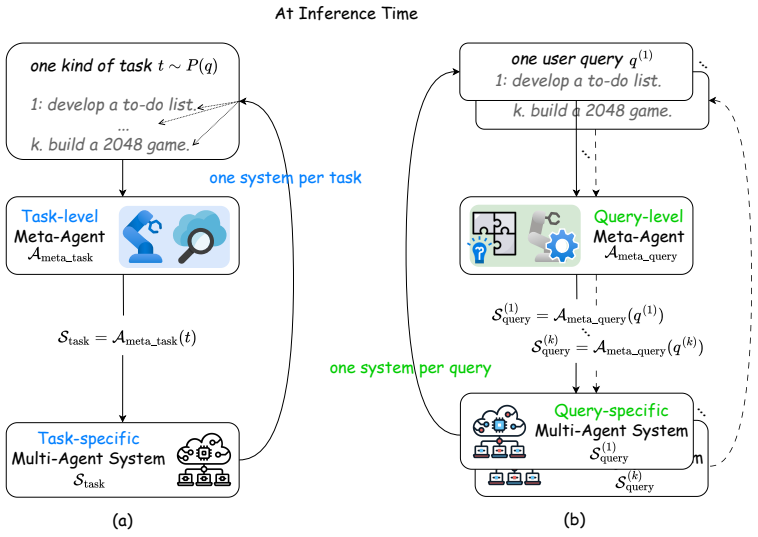


Figure 1: **Task-Level Meta-Agents vs. Query-Level Meta-Agents at Inference Time.** q denotes a user query, e.g., *build a 2048 game*. $t \sim P(q)$ denotes one kind of task, e.g., *code generation task*, which is a distribution of user queries. Given t, previous task-level meta-agent $\mathcal{A}_{\text{meta\_task}}$ aims to search a task-specific multi-agent system $\mathcal{S}_{\text{task}}$ to solve all queries sampled from t, i.e., one system per task. Differently, given one user query $q^{(i)}$, our query-level meta-agent $\mathcal{A}_{\text{meta\_query}}$ conducts reasoning and output a query-specific multi-agent system $\mathcal{S}^{(i)}_{\text{query}}$ for $q^{(i)}$, i.e., one system per query.

propose to integrate **external execution feedback** of the generated multi-agent system, based on which a **reasoning-driven meta-agent** is leveraged to polish the system.

We dub such a meta-agent as FlowReasoner. We first synthesize thousands of warm-up SFT data using DeepSeek R1-671B (Team, 2025a) as the meta-agent to generate multi-agent systems and process user queries individually. These synthetic data are then used to finetune DeepSeek-R1-Distill-Qwen-7B, enabling basic reasoning for multi-agent system generation. Furthermore, we enhance its reasoning capabilities for generating novel query-level multi-agent systems through reinforcement learning (RL), incorporating external execution feedback. A **multi-purpose reward** is designed to guide RL training, focusing on *performance*, *complexity*, and *efficiency*. During inference, FlowReasoner leverages deliberative reasoning to generate a novel query-level multi-agent system for each user query, achieving *one system per user query*. The main contributions are summarized as follows:

- We propose a query-level meta-agent termed FlowReasoner to automate the designs of query-level multi-agent systems, improving their adaptability in real-world scenarios.
- We train FlowReasoner to reason from external execution feedback via RL, guided by a multi-purpose reward considering performance, complexity, and efficiency.
- We demonstrate the superiority of FlowReasoner via extensive experiments and open-source it.

2 Problem Definition

We denote a user **query** as q, e.g., *build a 2048 game*. Then a user **task** is defined as a distribution of user queries, denoted as $t = P(q)$, e.g., *code generation task*. A multi-agent system is denoted as $\mathcal{S} = \{\mathcal{A}, \mathcal{W}\}$, where $\mathcal{A} = \{\mathcal{A}_1, ..., \mathcal{A}_n\}$ denotes the agents in the system and $\mathcal{W}$ is the *workflow* of collaboration among the agents.

As shown in Figure 2 (a), in traditional multi-agent systems (Hong et al., 2023; Wu et al., 2023; Li et al., 2023), the agents and the workflows are designed manually according to one kind of task $t = P(q)$, as formulated $\mathcal{S}_{\text{task}} = \mathcal{H}(t)$, where $\mathcal{H}$ denotes human experts, and $\mathcal{S}_{\text{task}}$ denotes the **task-level multi-agent system** which is fixed for all queries in one task. This kind of manually designed multi-agent system leads to extensive

human costs. Besides, such a one-size-fits-all system fails to allocate inference resources dynamically for different user queries within the task.

As illustrated in Figure 2 (b), search-based automatic multi-agent systems (Zhang et al., 2024b; Hu et al., 2024; Chen et al., 2023a) are proposed to reduce human effort. Specifically, these approaches first prompt an LLM, such as GPT-4o, to act as a meta-agent, generating multiple candidate multi-agent system designs. Subsequently, complex search algorithms are employed on the carefully designed search set to identify the optimal system for completing the task. We denote this kind of meta-agent as **task-level meta-agent** $\mathcal{A}_{\text{meta\_task}}$ since they can merely generate one **task-level multi-agent system** $\mathcal{S}_{\text{task}}$ to solve one kind of task t. Although effective, they are still one-size-fits-all systems. Besides, the search algorithm is time-consuming and relies on the search set, which is absent in one user query.

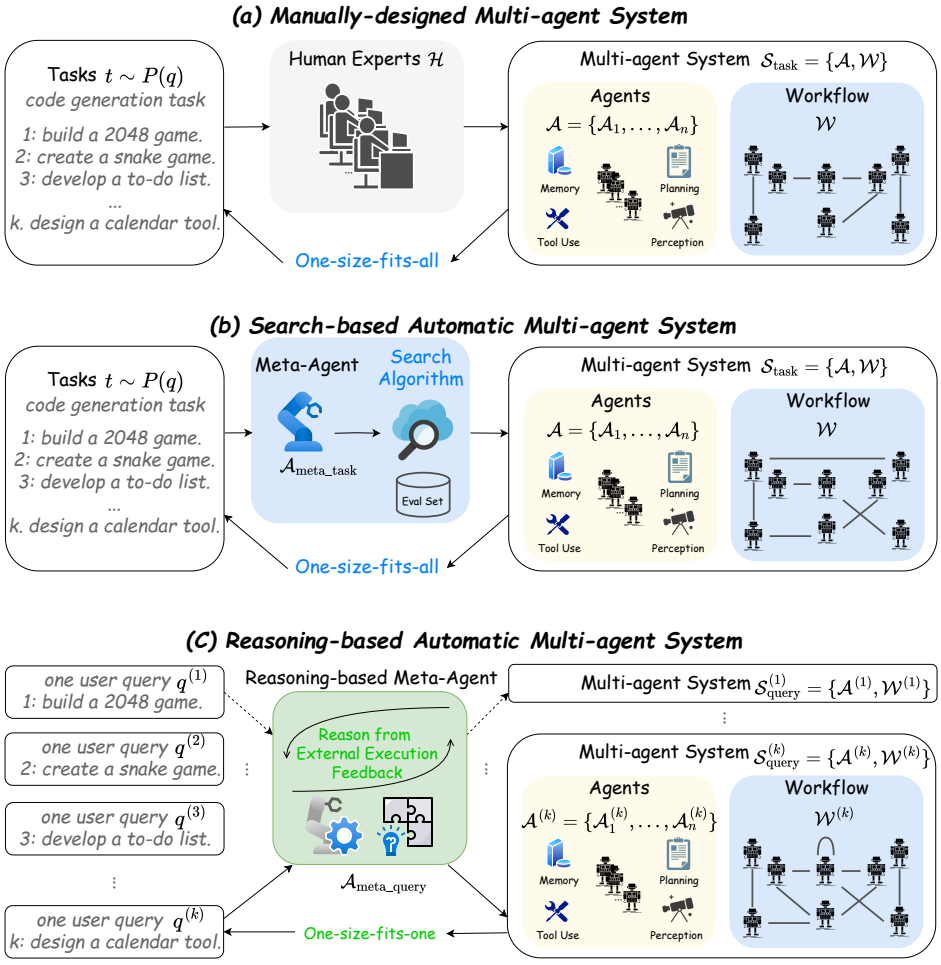


Figure 2: **Comparison of Three Multi-Agent Systems**. (a) Manually-designed Multi-agent System, (b) Search-based Automatic Multi-agent System, and (c) Reasoning-based Automatic Multi-agent System.

3 Meta-Agent FlowReasoner

To solve these problems, we develop a reasoning-based automatic multi-agent system shown in Figure 2 (c). Concretely, by guiding the model to reason from external execution feedback, we train a **query-level meta-agent** denoted as $\mathcal{A}_{\text{meta\_query}}$, which can automatically propose a novel **query-level multi-agent system** for each user query q, as formulated $\mathcal{S}_{\text{query}} = \mathcal{A}_{\text{meta\_query}}(q)$. Then, $\mathcal{S}_{\text{query}}$ accomplishes the specific user query and obtain the result a, i.e., $a = \mathcal{S}_{\text{query}}(q)$. Subsequently, the evaluator $\mathcal{E}$ evaluates the performance of the proposed multi-agents system $\mathcal{S}_{\text{query}}$ by comparing the result a with ground truth a_{gt} as formulated

Table 1: **Performance Evaluation.** Accuracy comparison across three code benchmarks for three categories of baselines - individual models, manual workflows, and automated workflow methods - alongside our FLOWREASONER-14B. For manual methods, model names in parentheses indicate the worker model used.

Type	Method	BigCodeBench	HumanEval	MBPP	Overall
Vanilla	o1-mini	57.67	95.42	74.19	71.37
	GPT-4o-mini	56.33	88.55	71.73	68.60
Manual	Self-Refine (4o-mini) (Madaan et al., 2023)	54.78	89.83	69.64	67.29
	LLM-Debate (4o-mini) (Du et al., 2023)	56.88	91.64	70.28	68.69
	LLM-Blender (4o-mini) (Jiang et al., 2023)	57.46	89.44	76.39	71.25
	Self-Refine (o1-mini) (Madaan et al., 2023)	56.68	94.74	73.64	70.63
	LLM-Debate (o1-mini) (Du et al., 2023)	57.25	95.83	74.28	71.33
	LLM-Blender (o1-mini) (Jiang et al., 2023)	59.51	96.37	78.65	74.22
Auto	AutoAgents (Chen et al., 2023a)	56.65	88.91	72.03	68.92
	ADAS (Hu et al., 2024)	53.87	84.26	68.47	65.48
	Aflow (Zhang et al., 2024b)	59.83	94.15	82.40	75.63
	MaAS (Zhang et al., 2025)	60.33	95.42	84.16	76.81
	ScoreFlow (Wang et al., 2025)	60.71	95.67	84.73	77.25
Ours	FLOWREASONER-14B	**63.53**	**97.26**	**92.15**	**81.89**

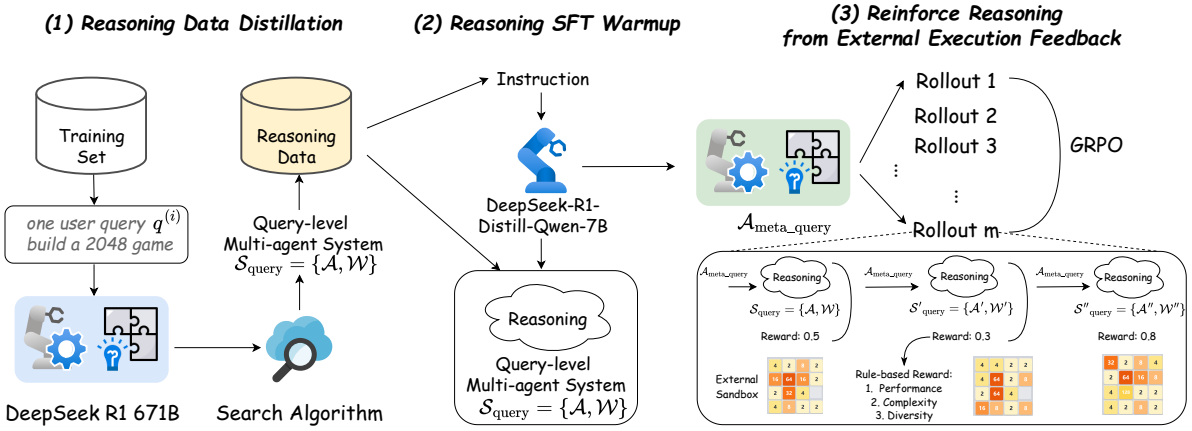


Figure 3: **Training Pipeline of FlowReasoner.** It consists of (1) Reasoning Data Distillation, (2) Reasoning SFT Warmup, (3) Reinforce Reasoning from external execution feedback.

$\mathcal{E}(a, a_{\text{gt}})$. Our proposed method is more practical in real-world scenarios, as it can design an optimal multi-agent system for each specific query. The training pipeline of our method is demonstrated in Figure 3.

3.1 Learn to Reason

Reasoning Data Syntheses. To enable our model to learn how to reason workflows based on external execution feedback, we first generate multi-round reasoning data using R1-671B(Team, 2025a). For a given input query q, the R1 model generates l rounds of reasoning $\mathcal{R}_{\text{query}}$ and a multi-agent system $\mathcal{S}_{\text{query}}$ with external execution feedback at each round as follows:

$$\{\{\mathcal{R}_{\text{query}}, \mathcal{S}_{\text{query}}\}^{(1)}, ..., \{\mathcal{R}_{\text{query}}, \mathcal{S}_{\text{query}}\}^{(l)}\} = \mathcal{A}_{\text{meta\_query}}(q). \tag{1}$$

Then, we concatenate the model's l rounds of reasoning and multi-agent system to form a reasoning process $\hat{\mathcal{R}}$ and final multi-agent system $\hat{\mathcal{S}}$, and pair it with the instruction $\mathcal{I}$ and query q to construct our training sample $\{\mathcal{I}, q, \hat{\mathcal{R}}, \hat{\mathcal{S}}\}$. Based on this, we construct a warmup SFT dataset $\mathcal{D}$.

Reasoning SFT Warmup. After creating the reasoning training dataset $\mathcal{D}$, we proceed to perform reasoning SFT for warmup. We input the instruction $\mathcal{I}$ and query q, then guide DeepSeek-R1-Distill-Qwen-7B to

output reasoning process $\hat{\mathcal{R}}$ and final multi-agent system $\hat{\mathcal{S}}$. It can be formulated as follows:

$$\mathcal{L}_{\text{SFT}} = -\mathbb{E}_{(\mathcal{I},q,\hat{\mathcal{R}},\hat{\mathcal{S}})\sim\mathcal{D}} \log P_\theta(\hat{\mathcal{R}}, \hat{\mathcal{S}} \mid \mathcal{I}, q), \tag{2}$$

where θ denotes the model parameters. Through SFT, we unlock the model's reasoning ability regarding workflow generation.

3.2 Reinforce Reasoning from External Execution Feedback

After the SFT stage, we use reinforcement learning phase to further enhance the model's reasoning capabilities through workflows built on external execution feedback. We aims to leverage feedback to improve performance on complex tasks in multi-round multi-agent systems. Following the DeepSeek-R1-Zero (Team, 2025a), we adopt standard GRPO (Grouped Relative Policy Optimization) as our training method. GRPO works by sampling multiple outputs for each query and computing relative advantages based on the rewards these outputs receive. The policy is then updated by maximizing an objective function incorporating these relative advantages. The GRPO objective function can be expressed as follows:

$$\begin{aligned}\mathcal{L}_{\text{GRPO}}(\theta) = \mathbb{E}_{q\sim t,\ \{o_i\}_{i=1}^{G}\sim\pi_{\theta_{\text{old}}}(O|q)} \\ \frac{1}{G}\sum_{i=1}^{G} \min[r_{\text{ratio}}, \text{clip}(r_{\text{ratio}}, 1-\varepsilon, 1+\varepsilon)] \cdot \hat{E}_{i,m} - \beta\, \mathbb{D}_{\text{KL}}(\pi_\theta \,\|\, \pi_{\text{ref}})\ .\end{aligned} \tag{3}$$

where G represents the number of sampled trajectories in each group, o_i denotes the i-th trajectory, $|o_i|$ is the length of trajectory o_i, $r_{\text{ratio}} = \frac{\pi_\theta(o_{i,m}|q,o_{i,<m})}{\pi_{\theta_{\text{old}}}(o_{i,m}|q,o_{i,<m})}$ represents the probability ratio between new and old policies, $\hat{E}_{i,m}$ is the estimated advantage for the m-th token in the i-th trajectory, ε is a small positive clipping parameter that prevents excessively large update steps, and the KL regularization term constrains policy drift to maintain stability during training.

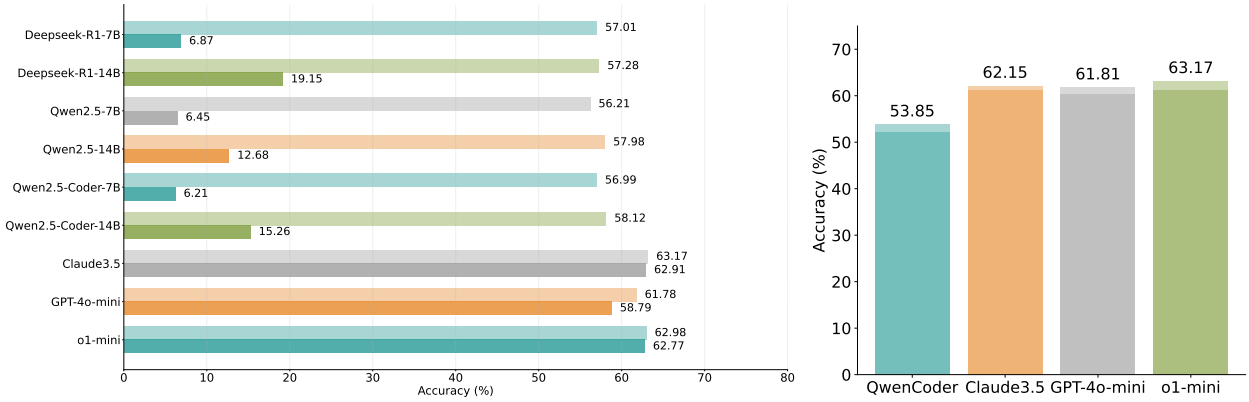
Since we can obtain a reward from the external environment in every round, we use process reward supervision. The reward for each reasoning round is normalized, and the advantage function is calculated as the sum of subsequent normalized rewards.

$$\hat{E}_{i,m} = \sum_{j\geq T} \tilde{r}_j^{(i)}. \tag{4}$$

Here, the normalized reward for the j-th round of the i-th candidate output is defined as $\tilde{r}_j^{(i)} = k^j \cdot \frac{r_j^{(i)} - \text{mean}(\mathbf{R})}{\text{std}(\mathbf{R})}$, where k is a scaling factor and T is a threshold used to exclude the first T items from the calculation. The set $\mathbf{R}$ represents the list of scores for each round across all candidates, and $r_j^{(i)}$ is the score of candidate i in round j. Each score $r_j^{(i)}$ is calculated by the performance of the proposed solution (i.e., pass rate), algorithm complexity (i.e., complexity score of abstract syntax tree) and diversity (i.e., distinctness ratio followed by Chen et al. (2024)) of workflow.

3.3 Generate Multi-Agent Systems with FlowReasoner

Constructing a multi-agent system is essentially an optimization problem with the goal of designing an optimized system, $\mathcal{S}^*_{\text{query}}$, that responds to user queries. When a user submits a query q, the system produces an answer $a = \mathcal{S}_{\text{query}}(q)$. The performance of the system in each round is evaluated using an external feedback function $\mathcal{E}(a, a_{\text{gt}})$, where a_{gt} represents the ground truth answer. In this framework, a meta-agent, $\mathcal{A}_{\text{meta\_query}}$, is responsible for optimizing the workflow with external execution feedback $\mathcal{E}(a, a_{\text{gt}})$ in every round. The pass rate of the proposed solution for the given query, as the key performance indicator of the system, serves as the external execution feedback. The optimization space is defined by all possible configurations of nodes and edges. Here, nodes represent various parameters (such as language models, prompts, temperature, and output formats), and edges capture the interactions or data flows between these nodes.



(a) Ablation of Meta-agent (b) Ablation of Workers

Figure 4: **Ablation of Meta-agent and Workers.** (a) Accuracy of different meta-agents with o1-mini as workers. (B) Accuracy of the generated workflow with different workers. The light bars show results with the initial workflow (multi-round iterations), while the dark bars show results without it.

Table 2: **Generalization Evaluation.** Accuracy of our trained meta-agent FlowReasoner-7B/14B when paired with alternative workers including Qwen2.5 Coder, Claude, and GPT4o-mini.

Worker/Meta-agent	FlowReasoner-7B (SFT+RL)			FlowReasoner-14B (SFT+RL)		
	BigCodeBench	HumanEval	MBPP	BigCodeBench	HumanEval	MBPP
o1-mini	62.77	96.95	89.86	63.53	97.26	92.15
Qwen2.5Coder-32b	50.17	92.89	80.40	52.67	93.69	78.90
Claude3.5	60.67	96.07	87.63	61.12	96.52	89.82
GPT-4o-mini	59.18	94.24	82.19	59.75	94.52	82.27

By representing both nodes and edges in code and employing predefined operators (such as Ensemble, Review, and Revise) along with a custom operator to combine these elements, FlowReasoner utilizes an l-round optimization process same as Aflow (Zhang et al., 2024b) to arrive at the final multi-agent system:

$$\mathcal{S}^*_{\text{query}} = \arg\max_{\mathcal{S}_{\text{query}} \in \mathbf{S}} \mathcal{E}(\mathcal{S}_{\text{query}}(q), a_{\text{gt}}), \tag{5}$$

where $\mathcal{S}^*_{\text{query}}$ is the optimal multi-agent system refined through optimization. By optimizing a multi-agent system through iterative external execution feedback, FlowReasoner can construct a highly adaptive system that maximizes the accuracy and performance of solution for a query.

4 Experiments

Datasets. Given our focus on creating workflows tailored to individual user queries rather than the general task, we restrict our scope to *code generation tasks*, as they can provide test cases as external execution feedback for the workflow construction process. Among various benchmarks, we consider three representative datasets: BigCodeBench (Zhuo et al., 2024), which emphasizes engineering-oriented tasks, and two algorithmically focused benchmarks, HumanEval (Chen et al., 2021) and MBPP (Austin et al., 2021). This selection enables us to comprehensively evaluate workflow discovery across a diverse spectrum of code generation challenges.

Baselines. In line with prior work (Hu et al., 2024; Zhang et al., 2024b), we evaluate FlowReasoner against three categories of baselines: (1) single-model direct invocation, where a single LLM is prompted to solve the problem without additional structure; (2) manually designed workflows, including Self-Refine (Madaan et al., 2023), LLM-Debate (Du et al., 2023), and LLM-Blender (Jiang et al., 2023), which incorporate human-crafted reasoning strategies; and (3) automated workflow optimization methods, such as Aflow (Zhang et al., 2024b), ADAS (Hu et al., 2024), and MaAS (Zhang et al., 2025), which construct workflows through search or

Table 3: **Ablation Study on Model Sizes and Training Stages.** Accuracy(%) comparison across three code benchmarks for models of different sizes (7B/14B) at both the Supervised Fine-Tuning (SFT) stage and the combined SFT with Reinforcement Learning (SFT+RL) stage.

Stage	Size	BigCodeBench	HumanEval	MBPP	Overall
SFT	7B	61.79	96.38	87.22	78.89
SFT+RL	7B	62.78	96.95	89.86	80.53
SFT	14B	62.83	97.18	91.91	81.50
SFT+RL	14B	63.53	97.26	92.15	81.89

optimization over possible reasoning structures. This comparison enables a comprehensive assessment of FlowReasoner's effectiveness relative to both static and adaptive baselines.

Implementation Details. For the manually designed workflow baselines, we employed both o1-mini and GPT-4o-mini as worker models for each method. For the automated workflow optimization baselines, we adopted the original configurations as described in MaAS (Zhang et al., 2025). In our proposed method, FlowReasoner, we trained two variants of DeepSeek-R1-Distill-Qwen with 7B and 14B parameters, respectively, and used o1-mini as the worker model. We fixed the number of workflow iterations to 10. To assess performance, we used the standard pass@1 metric for code accuracy, consistent with prior work (Chen et al., 2021). More details can be found in Appendix 7.

4.1 Experiment Results

Performance Comparison. Table 1 presents the performance comparison between our proposed method and the baselines. FlowReasoner-14B consistently outperforms all competing approaches across the three benchmark datasets. Notably, it achieves an overall improvement of 5 percentage points over the strongest baseline, MaAS, and exceeds the performance of its underlying worker model, o1-mini, by a substantial margin of 10%. These results highlight the effectiveness of our workflow-based reasoning framework in enhancing code generation accuracy.

Ablation on Model Size and Training Stages. To investigate the impact of model size and training stages on performance, we conducted an ablation study comparing different configurations of FlowReasoner in Table 3. We observed that the 14B variant consistently outperformed the 7B counterpart across all benchmarks, indicating a positive correlation between model scale and reasoning effectiveness. Furthermore, within each model size, versions trained with both SFT and RL exhibited notable improvements over those trained with SFT alone, demonstrating the complementary benefits of incorporating RL in enhancing workflow-guided code generation.

Ablation of Meta-agents and Workers. To analyze the impact of meta-agent and worker selection, we conducted an ablation study on the BigCodeBench dataset. Figure 4 presents performance comparisons under various meta-agent and worker configurations. As shown in Figure 4 (a), open-source models exhibited poor performance when paired with o1-mini as the worker and no initial workflow, frequently generating error-prone workflows. This highlights a limitation of current open-source models, which struggle to produce reliable workflows solely based on instruction prompts and are heavily reliant on predefined, manually crafted workflows. In contrast, API-based models demonstrated stronger performance, likely attributable to their superior instruction-following capabilities. Figure 4 (b) further examines worker effectiveness when using a high-performing meta-agent (Claude 3.5). We compared the open-source model Qwen2.5-Coder-32B and three API-based models, including Claude 3.5, GPT-4o-mini, and o1-mini. Among these, o1-mini achieved the best overall performance, suggesting its suitability as a worker model in the FlowReasoner framework.

Generalization Capability. To evaluate whether FlowReasoner, trained with o1-mini as the worker, can generalize its planning capabilities to alternative workers, we conducted experiments by substituting the worker with Qwen2.5-Coder, Claude, and GPT-4o-mini, while keeping the meta-agent fixed as either FlowReasoner-7B or FlowReasoner-14B. As shown in Table 2, FlowReasoner exhibits a notable degree of transferability, maintaining consistent performance across different worker models on the same

tasks. These results suggest that the planner is not tightly bound to a specific worker and can adapt its strategies effectively across diverse execution agents.

Case Study. Figure 5 illustrates two example workflows generated by FlowReasoner-14B for representative tasks from BigCodeBench and HumanEval, respectively. The workflow corresponding to the BigCodeBench task exhibits greater complexity, reflecting the more challenging and engineering-oriented nature of the task. In contrast, the HumanEval workflow is substantially more concise, aligning with the relative simplicity and algorithmic focus of the task. These examples demonstrate FlowReasoner 's ability to adapt the structure and granularity of workflows based on task complexity.

```python
async def __call__(self, problem: str, test_cases: list):
    max_retries = 3
    solutions = []

    for _ in range(max_retries):
        for attempt in range(3):
        # Try generating code up to 3 times
            solution = await self.custom_code_generate(
                problem=problem, instruction=prompt_custom.GENERATE_CODE_PROMPT
                )
            test_result = await self.test(
                problem=problem, solution=solution['response'], test_cases=test_cases
            )

            if test_result['result']:
                solutions.append(solution['response'])
                break  # Break the inner loop if a correct solution is found
            elif attempt < 2:
            # If it's not the last attempt, try to improve the solution
                error_analysis = await self.custom(
                input=f"Problem: {problem}\nFailed solution: {solution['response']}\nError: {
                    test_result['solution']}", instruction=prompt_custom.ERROR_ANALYSIS_PROMPT
                )
                prompt_custom.GENERATE_CODE_PROMPT = f"{prompt_custom.GENERATE_CODE_PROMPT}\n{
                    error_analysis['response']}"

        if not solutions:  # If no correct solution was found after 3 attempts
            solutions.append(solution['response'])  # Add the last generated solution

    best_solution = await self.sc_ensemble(solutions=solutions, problem=problem)
    return best_solution['response'], self.llm.cost_manager.total_cost
```

(a) Workflow generated by FlowReasoner-14B for the BigCodeBench task of *generating traffic data for various vehicle types over a specified number of hours, saving the data to a CSV file with columns, and plotting it in a line chart.*

```python
    async def __call__(self, problem: str, test_cases: list):
        solution = await self.custom_code_generate(problem=problem, entry_point=entry_point,
            instruction=prompt_custom.CODE_GENERATE_PROMPT)

        # Add review to check the solution
        review = await self.custom(
        input=f"Problem: {problem}\nGenerated solution: {solution['response']}", instruction=
            prompt_custom.REVIEW_PROMPT
        )

        # Improve the solution based on the review information
        improved_solution = await self.custom_code_generate(
        problem=problem, instruction=f"{prompt_custom.CODE_IMPROVE_PROMPT}\n\nConsider this review: {
            review['response']}"
        )

        return improved_solution['response'], self.llm.cost_manager.total_cost
```

(b) Workflow generated by FlowReasoner-14B for the HumanEval task of *splitting string into words and returning as an array.*

Figure 5: Cases of Workflows generated by FlowReasoner-14B for the tasks of BigCodeBench and HumanEval.

```python
async def __call__(self, problem: str, test_cases: list):
    # Extract key problem requirements and constraints
    problem_analysis = await self.custom(
        input=problem,
        instruction=prompt_custom.GRAPH_ANALYZE_PROMPT
    )

    # Generate initial solution with problem analysis context
    solution = await self.custom_code_generate(
        problem=problem,
        entry_point=entry_point,
        instruction=f"{prompt_custom.GRAPH_GENERATE_PROMPT}\nProblem Analysis: {problem_analysis['response']}"
    )

    current_solution = solution['response']

    # Loop for max_iterations to improve the solution if tests fail
    for iteration in range(3):
        # Test current solution
        test_results = await self.custom(
            input=f"Solution: {current_solution}\nTest Cases: {test_cases}",
            instruction=prompt_custom.GRAPH_TEST_PROMPT
        )

        # If tests pass, return the solution
        if "failed" not in test_results['response'].lower():
            return current_solution, self.llm.cost_manager.total_cost

        # Improve solution with test feedback and problem analysis
        improved_solution = await self.custom_code_generate(
            problem=problem,
            entry_point=entry_point,
            instruction=f"{prompt_custom.GRAPH_IMPROVE_PROMPT}\nProblem Analysis: {problem_analysis['response']}\nCurrent Solution: {current_solution}\nTest Results: {test_results['response']}\nIteration: {iteration + 1}/{max_iterations}"
        )

        # Update current solution
        current_solution = improved_solution['response']

    # Return the last solution attempt
    return current_solution, self.llm.cost_manager.total_cost
```

Figure 6: Successful workflow generated by FlowReasoner-14B for the BigCodeBench task of *Generating and plot weather data for a specified date range.*

```python
async def __call__(self, problem: str, test_cases: list):
    # Generate solution
    solution = await self.custom_code_generate(problem=problem, entry_point=entry_point, instruction=prompt_custom.GRAPH_GENERATE_PROMPT)

    # Test solution
    test_results = await self.custom(
        input=f"Solution: {solution['response']}\nTest Cases: {test_cases}",
        instruction=prompt_custom.GRAPH_TEST_PROMPT
    )

    # Optimize solution if tests fail
    if "failed" in test_results['response'].lower():
        improved_solution = await self.custom_code_generate(
            problem=problem,
            instruction=f"{prompt_custom.GRAPH_IMPROVE_PROMPT}\n\nTest Results: {test_results['response']}"
        )
        return improved_solution['response'], self.llm.cost_manager.total_cost

    return solution['response'], self.llm.cost_manager.total_cost
```

Figure 7: Successful workflow generated by FlowReasoner-14B for the MBPP task of *Writing a function to reverse words in a given string.*

```python
async def __call__(self, problem: str, test_cases: list):
    # 1. Prepare generation prompts
    gen_prompts = [
        prompt_custom.CODE_GENERATE_PROMPT_A,
        prompt_custom.CODE_GENERATE_PROMPT_B,
        prompt_custom.CODE_GENERATE_PROMPT_C,
    ]

    # 2. Generate three candidate solutions
    sols = [
        (await self.custom_code_generate(
            problem=problem,
            instruction=inst
        ))['response'] for inst in gen_prompts
    ]

    # 3. Ensemble: pick or merge the best solution
    ensemble_input = "Solutions:\n" + "\n---\n".join(sols)

    best = (await self.custom(
        input=ensemble_input,
        instruction=prompt_custom.ENSEMBLE_PROMPT
    ))['response']

    # 4. Return the best solution and total cost
    return best, self.llm.cost_manager.total_cost
```

Figure 8: Successful workflow generated by FlowReasoner-14B for the HumanEval task of *Returning list of prime factors of given integer in the order from smallest to largest.*

5 Related Work

LLM-Based Multi-Agent Systems. LLM-based multi-agent systems (Guo et al., 2024; Du et al., 2023; Chen et al., 2023b; Park et al., 2023; Huang et al., 2024; Jin et al., 2025; He et al., 2025b; 2026; 2025c;a; Hu et al., 2026) underpin many real-world applications, including code intelligence (CognitionAI, 2024), computer use (Anthropic, 2024), and deep research (OpenAI, 2025). These systems equip agents with planning, tool use, and database access, enabling collaborative problem solving.

Most existing systems rely on manually designed workflows, limiting scalability and increasing human effort. To reduce this burden, prior works automate agent design by optimizing prompts (Yuksekgonul et al., 2024; Li et al., 2026), hyper-parameters (Saad-Falcon et al., 2024), or agent profiles (Chen et al., 2023a; Yuan et al., 2024; Fernando et al., 2023). However, these methods typically optimize agents while keeping workflows fixed. To automate workflow design, recent studies model workflows as graphs or networks and optimize their structures (Li et al., 2024; Zhou et al., 2024b; Zhang et al., 2024c; Shang et al., 2024; Zhuge et al., 2023; 2024; Khattab et al., 2024; Liu et al., 2023; Zhang et al., 2024a; Feng et al., 2025). ADAS (Hu et al., 2024) and AFLOW (Zhang et al., 2024b) further represent workflows with executable code and optimize them using meta-agent search or MCTS, while MaAS (Zhang et al., 2025) and ScoreFlow (Wang et al., 2025) explore architecture search and DPO-based workflow generation.

We argue that these approaches are primarily *task-level* meta-agents, generating a single workflow for an entire task domain. As illustrated in Figure 1(a), such one-size-fits-all systems lack flexibility for diverse user queries. In contrast, this work proposes a *query-level* meta-agent that dynamically generates a query-specific multi-agent system for each user query, as shown in Figure 1(b).

Reasoning in LLMs. Reasoning is a core capability of LLMs, enabling them to emulate human-like deliberation. Early works such as Chain-of-Thought prompting (Wei et al., 2022; Kojima et al., 2022) improve reasoning by encouraging step-by-step thinking. Subsequent studies further enhance reasoning through self-correction (Kumar et al., 2024; Li et al., 2025a), self-critique (Ke et al., 2023), debate (Liang et al., 2023; Du et al., 2023), and plan-and-solve strategies (Wang et al., 2023). Other efforts explore latent-space reasoning (Hao et al., 2024; Goyal et al., 2023). OpenAI's o1 model demonstrates the effectiveness of test-time scaling for reasoning, inspiring o1-like models such as QwQ (Team, 2024c), QvQ (Team, 2024b), DeepSeek-R1 (Team, 2025a), and Kimi (Team, 2025b). OpenAI's o3 further achieves strong performance on the ARC-AGI

```python
async def __call__(self, problem: str, test_cases: list):
    # 1. Analyze the problem
    analysis = await self.custom(
        input=problem,
        instruction=prompt_custom.ANALYZE_PROMPT
    )

    # 2. Generate initial solution
    solution = await self.custom_code_generate(
        problem=problem,
        instruction=prompt_custom.GENERATE_PROMPT,
        context=analysis['response']
    )

    # 3. Test with a subset of test cases
    sample_tests = test_cases[:min(3, len(test_cases))]
    test_result = await self.custom(
        input=f"Solution:\n{solution['response']}\nTests:\n{sample_tests}",
        instruction=prompt_custom.TEST_PROMPT
    )

    # 4. Handle based on test results
    if "all passed" in test_result['response'].lower():
        # Optimize if all tests pass
        final = await self.custom_code_generate(
            problem=problem,
            instruction=prompt_custom.OPTIMIZE_PROMPT,
            context=f"Solution:\n{solution['response']}"
        )
        return final['response'], self.llm.cost_manager.total_cost
    else:
        # Fix issues if tests fail
        fixed = await self.custom_code_generate(
            problem=problem,
            instruction=prompt_custom.FIX_PROMPT,
            context=f"Solution:\n{solution['response']}\nTest results:\n{test_result['response']}"
        )
        return fixed['response'], self.llm.cost_manager.total_cost
```

Figure 9: Failed workflow generated by FlowReasoner-14B for the MBPP task of *Writing a function to count those characters which have vowels as their neighbors in the given string.*

```python
async def __call__(self, problem: str, test_cases: list):
    # 1. Generate solution
    solution = (await self.custom_code_generate(
        problem=problem,
        instruction=prompt_custom.CODE_GENERATE_PROMPT
    ))['response']

    # 2. Test and refine solution
    refined_solution = (await self.custom_code_generate(
        problem=problem,
        instruction=prompt_custom.REFINE_PROMPT,
        context=f"Initial solution:\n{solution}\n\nTest cases:\n{test_cases}"
    ))['response']

    # 3. Return the solution and total cost
    return refined_solution, self.llm.cost_manager.total_cost
```

Figure 10: Failed workflow generated by FlowReasoner-14B for the HumanEval task of *Evaluating whether the given number n can be written as the sum of exactly 4 positive even numbers.*

benchmark (ARC-AGI, 2024). Recent studies show that LLMs increasingly shift from intuitive System 1 processing to deliberative System 2 reasoning (Li et al., 2025b). Reasoning has also been shown to improve safety (Liu et al., 2025a) and reduce hallucinations (Gao et al., 2025). However, o1-like models may suffer from overthinking (Chen et al., 2024), motivating token-efficient reasoning methods (Liu et al., 2025b). In this work, we develop an o1-like reasoning model as a query-level meta-agent, eliminating the need for complex search algorithms and carefully designed search sets.

```python
async def __call__(self, problem: str, test_cases: list):
    # Extract key problem requirements and constraints with detailed specifications
    problem_analysis = await self.custom(
        input=problem,
        instruction=prompt_custom.GRAPH_ANALYZE_PROMPT
    )

    # Initial approach planning with appropriate algorithm selection
    algorithm_selection = await self.custom(
        input=f"Problem: {problem}\nAnalysis: {problem_analysis['response']}",
        instruction=prompt_custom.GRAPH_ALGORITHM_SELECTION_PROMPT
    )

    # Generate solution with problem analysis and algorithm selection
    solution = await self.custom_code_generate(
        problem=problem,
        entry_point=entry_point,
        instruction=f"{prompt_custom.GRAPH_GENERATE_PROMPT}\nProblem Analysis: {problem_analysis['response']}\nAlgorithm Selection: {algorithm_selection['response']}"
    )

    # Self-review for logical errors and optimization opportunities
    code_review = await self.custom(
        input=f"Code: {solution['response']}",
        instruction=prompt_custom.GRAPH_CODE_REVIEW_PROMPT
    )

    # Generate improved solution with comprehensive context
    improved_solution = await self.custom_code_generate(
        problem=problem,
        entry_point=entry_point,
        instruction=f"{prompt_custom.GRAPH_IMPROVE_PROMPT}\nProblem Analysis: {problem_analysis['response']}\nAlgorithm Selection: {algorithm_selection['response']}\nCode Review: {code_review['response']}"
    )

    # Add explanation to the solution
    solution_explanation = await self.custom(
        input=f"Solution: {improved_solution['response']}\nProblem: {problem}",
        instruction=prompt_custom.GRAPH_SOLUTION_EXPLANATION_PROMPT
    )

    final_solution = f"# Solution\n{improved_solution['response']}\n\n# Explanation\n{solution_explanation['response']}"
    return final_solution, self.llm.cost_manager.total_cost
```

Figure 11: Failed workflow generated by FlowReasoner-14B for the BigCodeBench task of *Extracting the text and href attributes of all anchor tags from a given URL's HTML content.*

6 Conclusion

We present FlowReasoner, a query-level meta-agent that automatically constructs personalized multi-agent workflows for individual queries. Unlike prior task-level approaches with fixed pipelines, FlowReasoner dynamically generates optimized workflows via reasoning-based optimization. It leverages external execution feedback and reinforcement learning with multi-objective rewards (performance, complexity, efficiency), avoiding complex search procedures. Experiments show that FlowReasoner-14B consistently outperforms both manual and automated baselines across code generation benchmarks, improving o1-mini by 10.52% overall. Results across different worker models further demonstrate strong generalization. Overall, FlowReasoner reduces human effort while enabling scalable, adaptive multi-agent systems tailored to each query.

7 Limitation

Despite demonstrating superior performance over existing approaches, FlowReasoner faces the limitation of the need for training, which needs some computational cost. Besides, while some generalization capability is shown when switching worker agent, performance still varies based on the worker agent used, suggesting partial dependency of the trained meta-agent on the underlying execution agent.

References

Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, et al. Gpt-4 technical report. *arXiv preprint arXiv:2303.08774*, 2023.

Anthropic. Introducing computer use, a new claude 3.5 sonnet, and claude 3.5 haiku. *https://www.anthropic.com/news/3-5-models-and-computer-use*, 2024.

ARC-AGI. Abstraction and reasoning corpus for artificial general intelligence. *https://github.com/fchollet/ARC-AGI/*, 2024.

Jacob Austin, Augustus Odena, Maxwell Nye, Maarten Bosma, Henryk Michalewski, David Dohan, Ellen Jiang, Carrie Cai, Michael Terry, Quoc Le, et al. Program synthesis with large language models. *arXiv preprint arXiv:2108.07732*, 2021.

Guangyao Chen, Siwei Dong, Yu Shu, Ge Zhang, Jaward Sesay, Börje F Karlsson, Jie Fu, and Yemin Shi. Autoagents: A framework for automatic agent generation. *arXiv preprint arXiv:2309.17288*, 2023a.

Mark Chen, Jerry Tworek, Heewoo Jun, Qiming Yuan, Henrique Ponde De Oliveira Pinto, Jared Kaplan, Harri Edwards, Yuri Burda, Nicholas Joseph, Greg Brockman, et al. Evaluating large language models trained on code. *arXiv preprint arXiv:2107.03374*, 2021.

Weize Chen, Yusheng Su, Jingwei Zuo, Cheng Yang, Chenfei Yuan, Chen Qian, Chi-Min Chan, Yujia Qin, Yaxi Lu, Ruobing Xie, et al. Agentverse: Facilitating multi-agent collaboration and exploring emergent behaviors in agents. *arXiv preprint arXiv:2308.10848*, 2(4):6, 2023b.

Xingyu Chen, Jiahao Xu, Tian Liang, Zhiwei He, Jianhui Pang, Dian Yu, Linfeng Song, Qiuzhi Liu, Mengfei Zhou, Zhuosheng Zhang, et al. Do not think that much for 2+ 3=? on the overthinking of o1-like llms. *arXiv preprint arXiv:2412.21187*, 2024.

CognitionAI. Introducing devin, the first ai software engineer. *https://www.cognition.ai/blog/introducing-devin/*, 2024.

Yilun Du, Shuang Li, Antonio Torralba, Joshua B Tenenbaum, and Igor Mordatch. Improving factuality and reasoning in language models through multiagent debate, 2023. *URL https://arxiv. org/abs/2305.14325*, 3, 2023.

Shangbin Feng, Zifeng Wang, Palash Goyal, Yike Wang, Weijia Shi, Huang Xia, Hamid Palangi, Luke Zettlemoyer, Yulia Tsvetkov, Chen-Yu Lee, et al. Heterogeneous swarms: Jointly optimizing model roles and weights for multi-llm systems. *arXiv preprint arXiv:2502.04510*, 2025.

Chrisantha Fernando, Dylan Banarse, Henryk Michalewski, Simon Osindero, and Tim Rocktäschel. Promptbreeder: Self-referential self-improvement via prompt evolution. *arXiv preprint arXiv:2309.16797*, 2023.

Hongcheng Gao, Jiashu Qu, Jingyi Tang, Baolong Bi, Yue Liu, Hongyu Chen, Li Liang, Li Su, and Qingming Huang. Exploring hallucination of large multimodal models in video understanding: Benchmark, analysis and mitigation. *arXiv preprint arXiv:2503.19622*, 2025.

Sachin Goyal, Ziwei Ji, Ankit Singh Rawat, Aditya Krishna Menon, Sanjiv Kumar, and Vaishnavh Nagarajan. Think before you speak: Training language models with pause tokens. *arXiv preprint arXiv:2310.02226*, 2023.

Taicheng Guo, Xiuying Chen, Yaqi Wang, Ruidi Chang, Shichao Pei, Nitesh V Chawla, Olaf Wiest, and Xiangliang Zhang. Large language model based multi-agents: A survey of progress and challenges. *arXiv preprint arXiv:2402.01680*, 2024.

Shibo Hao, Sainbayar Sukhbaatar, DiJia Su, Xian Li, Zhiting Hu, Jason Weston, and Yuandong Tian. Training large language models to reason in a continuous latent space. *arXiv preprint arXiv:2412.06769*, 2024.

Yufei He, Ruoyu Li, Alex Chen, Yue Liu, Yulin Chen, Yuan Sui, Cheng Chen, Yi Zhu, Luca Luo, Frank Yang, et al. Enabling self-improving agents to learn at test time with human-in-the-loop guidance. In *Proceedings of the 2025 Conference on Empirical Methods in Natural Language Processing: Industry Track*, pp. 1625–1653, 2025a.

Yufei He, Yuexin Li, Jiaying Wu, Yuan Sui, Yulin Chen, and Bryan Hooi. Evaluating the paperclip maximizer: Are rl-based language models more likely to pursue instrumental goals? *arXiv preprint arXiv:2502.12206*, 2025b.

Yufei He, Juncheng Liu, Yue Liu, Yibo Li, Tri Cao, Zhiyuan Hu, Xinxing Xu, and Bryan Hooi. Evotest: Evolutionary test-time learning for self-improving agentic systems. *arXiv preprint arXiv:2510.13220*, 2025c.

Yufei He, Yuan Sui, Xiaoxin He, and Bryan Hooi. Unigraph: Learning a unified cross-domain foundation model for text-attributed graphs. In *Proceedings of the 31st ACM SIGKDD Conference on Knowledge Discovery and Data Mining V. 1*, pp. 448–459, 2025d.

Yufei He, Yuan Sui, Xiaoxin He, Yue Liu, Yifei Sun, and Bryan Hooi. Unigraph2: Learning a unified embedding space to bind multimodal graphs. In *Proceedings of the ACM on Web Conference 2025*, pp. 1759–1770, 2025e.

Yufei He, Juncheng Liu, Zhiyuan Hu, Yulin Chen, Yue Liu, Yuan Sui, Yibo Li, Nuo Chen, Jun Hu, Bryan Hooi, et al. Evoclinician: A self-evolving agent for multi-turn medical diagnosis via test-time evolutionary learning. *arXiv preprint arXiv:2601.22964*, 2026.

Sirui Hong, Xiawu Zheng, Jonathan Chen, Yuheng Cheng, Jinlin Wang, Ceyao Zhang, Zili Wang, Steven Ka Shing Yau, Zijuan Lin, Liyang Zhou, et al. Metagpt: Meta programming for multi-agent collaborative framework. *arXiv preprint arXiv:2308.00352*, 3(4):6, 2023.

Shengran Hu, Cong Lu, and Jeff Clune. Automated design of agentic systems. *arXiv preprint arXiv:2408.08435*, 2024.

Zhiyuan Hu, Yucheng Wang, Yufei He, Jiaying Wu, Yilun Zhao, See-Kiong Ng, Cynthia Breazeal, Anh Tuan Luu, Hae Won Park, and Bryan Hooi. Rewarding the rare: Uniqueness-aware rl for creative problem solving in llms. *arXiv preprint arXiv:2601.08763*, 2026.

Yichong Huang, Xiaocheng Feng, Baohang Li, Yang Xiang, Hui Wang, Ting Liu, and Bing Qin. Ensemble learning for heterogeneous large language models with deep parallel collaboration. In A. Globerson, L. Mackey, D. Belgrave, A. Fan, U. Paquet, J. Tomczak, and C. Zhang (eds.), *Advances in Neural Information Processing Systems*, volume 37, pp. 119838–119860. Curran Associates, Inc., 2024.

Dongfu Jiang, Xiang Ren, and Bill Yuchen Lin. Llm-blender: Ensembling large language models with pairwise ranking and generative fusion. *arXiv preprint arXiv:2306.02561*, 2023.

Can Jin, Hongwu Peng, Qixin Zhang, Yujin Tang, Dimitris N Metaxas, and Tong Che. Two heads are better than one: Test-time scaling of multi-agent collaborative reasoning. *arXiv preprint arXiv:2504.09772*, 2025.

Pei Ke, Bosi Wen, Zhuoer Feng, Xiao Liu, Xuanyu Lei, Jiale Cheng, Shengyuan Wang, Aohan Zeng, Yuxiao Dong, Hongning Wang, et al. Critiquellm: Scaling llm-as-critic for effective and explainable evaluation of large language model generation. *arXiv preprint arXiv:2311.18702*, 2023.

Omar Khattab, Arnav Singhvi, Paridhi Maheshwari, Zhiyuan Zhang, Keshav Santhanam, Saiful Haq, Ashutosh Sharma, Thomas T Joshi, Hanna Moazam, Heather Miller, et al. Dspy: Compiling declarative language model calls into state-of-the-art pipelines. In *The Twelfth International Conference on Learning Representations*, 2024.

Moo Jin Kim, Karl Pertsch, Siddharth Karamcheti, Ted Xiao, Ashwin Balakrishna, Suraj Nair, Rafael Rafailov, Ethan Foster, Grace Lam, Pannag Sanketi, et al. Openvla: An open-source vision-language-action model. *arXiv preprint arXiv:2406.09246*, 2024.

Takeshi Kojima, Shixiang Shane Gu, Machel Reid, Yutaka Matsuo, and Yusuke Iwasawa. Large language models are zero-shot reasoners. *Advances in neural information processing systems*, 35:22199–22213, 2022.

Aviral Kumar, Vincent Zhuang, Rishabh Agarwal, Yi Su, John D Co-Reyes, Avi Singh, Kate Baumli, Shariq Iqbal, Colton Bishop, Rebecca Roelofs, et al. Training language models to self-correct via reinforcement learning. *arXiv preprint arXiv:2409.12917*, 2024.

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, 2023.

Yibo Li, Miao Xiong, Jiaying Wu, and Bryan Hooi. Conftuner: Training large language models to express their confidence verbally. *arXiv preprint arXiv:2508.18847*, 2025a.

Yibo Li, Zijie Lin, Ailin Deng, Xuan Zhang, Yufei He, Shuo Ji, Tri Cao, and Bryan Hooi. Just-in-time reinforcement learning: Continual learning in llm agents without gradient updates. *arXiv preprint arXiv:2601.18510*, 2026.

Zelong Li, Shuyuan Xu, Kai Mei, Wenyue Hua, Balaji Rama, Om Raheja, Hao Wang, He Zhu, and Yongfeng Zhang. Autoflow: Automated workflow generation for large language model agents. *arXiv preprint arXiv:2407.12821*, 2024.

Zhong-Zhi Li, Duzhen Zhang, Ming-Liang Zhang, Jiaxin Zhang, Zengyan Liu, Yuxuan Yao, Haotian Xu, Junhao Zheng, Pei-Jie Wang, Xiuyi Chen, et al. From system 1 to system 2: A survey of reasoning large language models. *arXiv preprint arXiv:2502.17419*, 2025b.

Tian Liang, Zhiwei He, Wenxiang Jiao, Xing Wang, Yan Wang, Rui Wang, Yujiu Yang, Shuming Shi, and Zhaopeng Tu. Encouraging divergent thinking in large language models through multi-agent debate. *arXiv preprint arXiv:2305.19118*, 2023.

Aixin Liu, Bei Feng, Bing Xue, Bingxuan Wang, Bochao Wu, Chengda Lu, Chenggang Zhao, Chengqi Deng, Chenyu Zhang, Chong Ruan, et al. Deepseek-v3 technical report. *arXiv preprint arXiv:2412.19437*, 2024.

Yue Liu, Hongcheng Gao, Shengfang Zhai, Jun Xia, Tianyi Wu, Zhiwei Xue, Yulin Chen, Kenji Kawaguchi, Jiaheng Zhang, and Bryan Hooi. Guardreasoner: Towards reasoning-based llm safeguards. *arXiv preprint arXiv:2501.18492*, 2025a.

Yue Liu, Jiaying Wu, Yufei He, Hongcheng Gao, Hongyu Chen, Baolong Bi, Jiaheng Zhang, Zhiqi Huang, and Bryan Hooi. Efficient inference for large reasoning models: A survey. *arXiv preprint arXiv:2503.23077*, 2025b.

Zijun Liu, Yanzhe Zhang, Peng Li, Yang Liu, and Diyi Yang. Dynamic llm-agent network: An llm-agent collaboration framework with agent team optimization. *arXiv preprint arXiv:2310.02170*, 2023.

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. *Advances in Neural Information Processing Systems*, 36:46534–46594, 2023.

OpenAI. Introducing chatgpt. *https://openai.com/index/chatgpt/*, 2022.

OpenAI. Learning to reason with llms. *https://openai.com/index/learning-to-reason-with-llms/*, 2024.

OpenAI. Introducing deep research. *https://openai.com/index/introducing-deep-research/*, 2025.

Joon Sung Park, Joseph O'Brien, Carrie Jun Cai, Meredith Ringel Morris, Percy Liang, and Michael S Bernstein. Generative agents: Interactive simulacra of human behavior. In *Proceedings of the 36th annual acm symposium on user interface software and technology*, pp. 1–22, 2023.

Machel Reid, Nikolay Savinov, Denis Teplyashin, Dmitry Lepikhin, Timothy Lillicrap, Jean-baptiste Alayrac, Radu Soricut, Angeliki Lazaridou, Orhan Firat, Julian Schrittwieser, et al. Gemini 1.5: Unlocking multimodal understanding across millions of tokens of context. *arXiv preprint arXiv:2403.05530*, 2024.

Jon Saad-Falcon, Adrian Gamarra Lafuente, Shlok Natarajan, Nahum Maru, Hristo Todorov, Etash Guha, E Kelly Buchanan, Mayee Chen, Neel Guha, Christopher Ré, et al. Archon: An architecture search framework for inference-time techniques. *arXiv preprint arXiv:2409.15254*, 2024.

Yu Shang, Yu Li, Keyu Zhao, Likai Ma, Jiahe Liu, Fengli Xu, and Yong Li. Agentsquare: Automatic llm agent search in modular design space. *arXiv preprint arXiv:2410.06153*, 2024.

Anthropic Team. The claude 3 model family: Opus, sonnet, haiku. *https://www-cdn.anthropic.com/de8ba9b01c9ab7cbabf5c33b80b7bbc618857627/Model_Card_Claude_3.pdf*, 2024a.

Deepseek Team. Deepseek-r1: Incentivizing reasoning capability in llms via reinforcement learning. *arXiv preprint arXiv:2501.12948*, 2025a.

Kimi Team. Kimi k1.5: Scaling reinforcement learning with llms. *arXiv preprint 2501.12599v1*, 2025b.

Qwen Team. Qvq: To see the world with wisdom. *https://qwenlm.github.io/blog/qvq-72b-preview/*, 2024b.

Qwen Team. Qwq: Reflect deeply on the boundaries of the unknown. *https://qwenlm.github.io/blog/qwq-32b-preview/*, 2024c.

Lei Wang, Wanyu Xu, Yihuai Lan, Zhiqiang Hu, Yunshi Lan, Roy Ka-Wei Lee, and Ee-Peng Lim. Plan-and-solve prompting: Improving zero-shot chain-of-thought reasoning by large language models. *arXiv preprint arXiv:2305.04091*, 2023.

Yinjie Wang, Ling Yang, Guohao Li, Mengdi Wang, and Bryon Aragam. Scoreflow: Mastering llm agent workflows via score-based preference optimization. *arXiv preprint arXiv:2502.04306*, 2025.

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.

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

An Yang, Baosong Yang, Beichen Zhang, Binyuan Hui, Bo Zheng, Bowen Yu, Chengyuan Li, Dayiheng Liu, Fei Huang, Haoran Wei, et al. Qwen2. 5 technical report. *arXiv preprint arXiv:2412.15115*, 2024.

Chengrun Yang, Xuezhi Wang, Yifeng Lu, Hanxiao Liu, Quoc V Le, Denny Zhou, and Xinyun Chen. Large language models as optimizers. *arXiv preprint arXiv:2309.03409*, 2023.

Siyu Yuan, Kaitao Song, Jiangjie Chen, Xu Tan, Dongsheng Li, and Deqing Yang. Evoagent: Towards automatic multi-agent generation via evolutionary algorithms. *arXiv preprint arXiv:2406.14228*, 2024.

Mert Yuksekgonul, Federico Bianchi, Joseph Boen, Sheng Liu, Zhi Huang, Carlos Guestrin, and James Zou. Textgrad: Automatic" differentiation" via text. *arXiv preprint arXiv:2406.07496*, 2024.

Guibin Zhang, Yanwei Yue, Xiangguo Sun, Guancheng Wan, Miao Yu, Junfeng Fang, Kun Wang, and Dawei Cheng. G-designer: Architecting multi-agent communication topologies via graph neural networks. *arXiv preprint arXiv:2410.11782*, 2024a.

Guibin Zhang, Luyang Niu, Junfeng Fang, Kun Wang, Lei Bai, and Xiang Wang. Multi-agent architecture search via agentic supernet. *arXiv preprint arXiv:2502.04180*, 2025.

Jiayi Zhang, Jinyu Xiang, Zhaoyang Yu, Fengwei Teng, Xionghui Chen, Jiaqi Chen, Mingchen Zhuge, Xin Cheng, Sirui Hong, Jinlin Wang, et al. Aflow: Automating agentic workflow generation. *arXiv preprint arXiv:2410.10762*, 2024b.

Shaokun Zhang, Jieyu Zhang, Jiale Liu, Linxin Song, Chi Wang, Ranjay Krishna, and Qingyun Wu. Offline training of language model agents with functions as learnable weights. In *Forty-first International Conference on Machine Learning*, 2024c.

Yaowei Zheng, Richong Zhang, Junhao Zhang, Yanhan Ye, Zheyan Luo, Zhangchi Feng, and Yongqiang Ma. Llamafactory: Unified efficient fine-tuning of 100+ language models. *arXiv preprint arXiv:2403.13372*, 2024.

Pei Zhou, Jay Pujara, Xiang Ren, Xinyun Chen, Heng-Tze Cheng, Quoc V Le, Ed Chi, Denny Zhou, Swaroop Mishra, and Huaixiu Steven Zheng. Self-discover: Large language models self-compose reasoning structures. *Advances in Neural Information Processing Systems*, 37:126032–126058, 2024a.

Wangchunshu Zhou, Yixin Ou, Shengwei Ding, Long Li, Jialong Wu, Tiannan Wang, Jiamin Chen, Shuai Wang, Xiaohua Xu, Ningyu Zhang, et al. Symbolic learning enables self-evolving agents. *arXiv preprint arXiv:2406.18532*, 2024b.

Mingchen Zhuge, Haozhe Liu, Francesco Faccio, Dylan R Ashley, Róbert Csordás, Anand Gopalakrishnan, Abdullah Hamdi, Hasan Abed Al Kader Hammoud, Vincent Herrmann, Kazuki Irie, et al. Mindstorms in natural language-based societies of mind. *arXiv preprint arXiv:2305.17066*, 2023.

Mingchen Zhuge, Wenyi Wang, Louis Kirsch, Francesco Faccio, Dmitrii Khizbullin, and Jürgen Schmidhuber. Gptswarm: Language agents as optimizable graphs. In *Forty-first International Conference on Machine Learning*, 2024.

Terry Yue Zhuo, Minh Chien Vu, Jenny Chim, Han Hu, Wenhao Yu, Ratnadira Widyasari, Imam Nur Bani Yusuf, Haolan Zhan, Junda He, Indraneil Paul, et al. Bigcodebench: Benchmarking code generation with diverse function calls and complex instructions. *arXiv preprint arXiv:2406.15877*, 2024.

Implementation Details

In the workflow optimization process of our method, we evaluate each workflow for 3 times as external execution feedback. We use the following 6 operators based on Aflow (Zhang et al., 2024b) as our base operators:

- Code Generator: generates code solutions for a given problem.
- Format Generator: produces formatted answers for a given problem.
- Ensemble Operator: combines multiple solutions or approaches to create a more robust final result.
- Review Operator: evaluates solutions for correctness, efficiency, and adherence to requirements.
- Revise Operator: refines solutions based on feedback from the review process.
- Code Test Operator: executes and validates code solutions against test cases to ensure functionality.

For our supervised fine-tuning (SFT), we utilized approximately 1,400 items sourced from three datasets generated by R1 through our optimization process. We conducted the training using LLaMA-Factory (Zheng et al., 2024), with a per-device training batch size of 1, gradient accumulation over 2 steps, a learning rate of 1e-5, and max train epochs of 3. For the reinforcement learning (RL) phase, we set the scaling factor k to 1.1, the threshold T to 3, rollout number m to 5, and max episodes to 5. All experiments are conducted on NVIDIA A100 GPUs with 80GB of memory. The total cost of training stage is about 150 GPU hours.

The multi-purpose reward in RL is designed to balance correctness, efficiency, and exploration. However, both diversity and complexity rewards showed minimal improvement in accuracy-driven benchmarks. Consequently, we set the coefficients for these two rewards to 0.