Agent-Environment Alignment via Automated Interface Generation

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Abstract

Large language model agents have shown impressive capabilities in interactive decision-making tasks. These agents interact with environment through intermediate interfaces, such as predefined action spaces and interaction rules, which mediate the perception and action. However, mismatches often happen between the internal expectations of the agent regarding the influence of its issued actions and the actual state transitions in the environment, a phenomenon referred to as **agent-environment misalignment**. While prior work has invested substantially in improving agent strategies and environment design, the critical role of the interface still remains underexplored. In this work, we empirically demonstrate that agent-environment misalignment poses a significant bottleneck to agent performance. To mitigate this issue, we propose **ALIGN**, an Auto-Aligned Interface Generation framework that alleviates the misalignment by enriching the interface. Implemented as a lightweight wrapper, ALIGN-generated interface achieves the alignment without modifying either the agent logic or the environment code. Experiments across multiple domains including embodied tasks, web navigation and tool-use, achieve consistent performance improvements, with a 45.67% success rate improvement in ALFWorld.

1 Introduction

Large Language Model (LLM) agents have demonstrated promising performance in interactive tasks such as embodied tasks (Wang et al., 2024a), web navigation tasks (Qi et al., 2024), and tool-use tasks (Schick et al., 2023). In these tasks, agents typically interact with the environment through manually designed **interfaces** such as predefined action spaces and interaction rules. While substantial efforts have been devoted to improving agents and environments, comparatively little attention has been paid to the interface between them, leading to a problem we term **agent-environment misalignment**, which impacts the agent performance.

The agent-environment misalignment refers to the discrepancy between the interpretation of the agent to the observation following an action and the underlying logic of the environment. As illustrated in Figure 1 (left), in ALFWorld (Shridhar et al., 2021), an invalid action returns "Nothing happens", which agents misinterpret as an empty state rather than a constraint violation. This misalignment significantly hinders task success and imposes unnecessary cognitive overhead on agents. From the perspective of the agent, poorly designed interfaces impose unnecessary cognitive overhead. Furthermore, from an evaluation perspective, inadequate interfaces can obscure an accurate assessment of the true reasoning capabilities of agents. Therefore, we argue that the problem of agent-environment misalignment warrants greater attention.

However, addressing the agent-environment misalignment is challenging. On one hand, current benchmarks primarily focus on advance agent intelligence by constructing increasingly complex and challenging environments (Xie et al., 2024; Zhou et al., 2024a), often overlooking the importance of improving interface design. This oversight extends across multiple domains of interactive tasks, such as, ALFWorld, OSWorld (Xie et al., 2024), and M^3ToolEval (Wang et al., 2024b). They all exhibit similar deficiencies: failing to provide agent-parseable observations for environmental constraints violation in embodied tasks, positional inaccuracies in operating system tasks or parameter format errors in multi-turn tool-use tasks, respectively. On the other hand, although some recent work (Yang et al., 2024a; Zheng et al., 2024) has begun to consider interface design, these efforts often rely on manual, environment-specific tailoring, which introduces two critical issues: (1) they are highly labor-intensive and (2) whether human-designed interfaces are optimal for agents remains

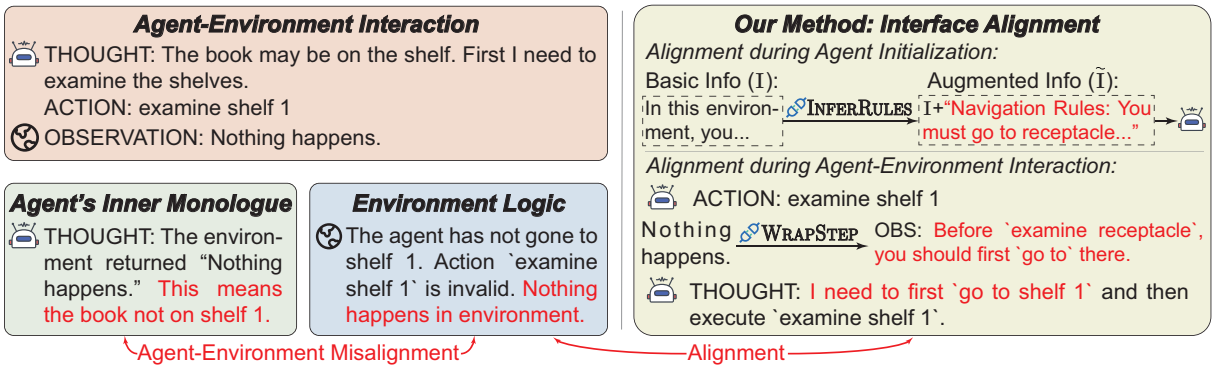

Figure 1: **Illustration of agent-environment misalignment and our proposed solution. Left:** The agent and the environment have a misalignment in their interpretation of the same observation, where the agent's understanding of the observation differs from the environment's underlying logic. **Right:** ALIGN bridges this gap via an automatically generated interface comprising two modules, **INFERRULES** and **WRAPSTEP**: (1) During initialization, INFERRULES augments the basic information with explicit environment constraints. (2) During interaction, WRAPSTEP translates the raw observation into an informative observation.

an open question. Furthermore, researchers often manually re-engineer interfaces for specific methods (Ma et al., 2024; Chen et al., 2024a), compromising comparability and making it unclear whether improvements stem from novel architectures or customized interfaces.

Distinct from the aforementioned works, we propose to **automatically generate interfaces for bridging the agent-environment misalignment**. In this work, we introduce **ALIGN** (Auto-Aligned Interface Generation), a framework that automatically generate aligned interfaces for environments. The generated interface consists of two modules: INFERRULES and WRAPSTEP. The former discovers and provides the agent with static information about environmental rules or internal constraints, facilitating *static alignment*, while the latter enhances the interaction by offering more detailed observations for agent-issuing actions, enabling *dynamic alignment*, as shown in Figure 1 (right). The generated interface acts as a lightweight wrapper, providing richer context and explicit constraint hints, enabling different LLM agents to align with the environment directly.

To evaluate the effectiveness of ALIGN, we conduct experiments on four representative benchmarks across three domains: embodied tasks, web navigation, and tool-use tasks. Our results demonstrate consistent performance improvements across all four benchmarks when using the ALIGN-generated interface, with notably gains of 45.67% in average success rate on ALFWorld. Moreover, the performance of GPT-4.1-based agents on ALFWorld are improved from 73.88% to 93.28% with ALIGN, highlighting the efficiency of our approach in mitigating the agent-environment misalignment to unleash the agent's true capabilities.

Our contributions are summarized as follows:

- We identify and characterize the **agent-environment misalignment**, empirically showing its prevalence across diverse domains and its role as a key bottleneck to performance.
- We introduce **ALIGN**, the first framework that automatically generates aligned interfaces to alleviate agent-environment misalignment, without modifying agent logic or environment code.
- We demonstrate the effectiveness and generalizability of **ALIGN** across three domains, with up to a 45.67% success rate gain on ALFWorld.

2 Related Work

Agent-environment interface The agent-environment interface defines how agents interact with the environment. In reinforcement learning, unified interaction interfaces (Bonnet et al., 2024; Brockman et al., 2016; Kolve et al., 2017; Towers et al., 2024) standardize the evaluation of different algorithms. As LLMs become increasingly capable of human-like actions (Guo et al., 2024; Liu et al., 2024; Ma et al., 2024), interface design has been shown to largely influence LLM-based agent performance (Xie et al., 2024; Rawles et al., 2024). SWE-agent (Yang et al., 2024a) proposes agent-computer interfaces for coding agents, and recent efforts aim to improve generalization (Agashe et al., 2024; Qin et al., 2025; Niu et al., 2024) or augment interfaces with auxiliary tools (Bula

et al., 2025; Gou et al., 2024; Lei et al., 2025; Lu et al., 2024; Yang et al., 2023a). However, these interfaces are mostly hand-crafted for specific environments or frameworks, limiting their generalization and scalability. We instead propose automated interface generation for effective, generalizable alignment.

Methods aligning agents with environments LLM agents have shown strong potential for real-world interaction and task completion (Yao et al., 2023; Shinn et al., 2023; Liu et al., 2024), with existing work falling into training-based and training-free categories. Training-based methods fine-tune LLMs on expert trajectories (Zeng et al., 2024; Chen et al., 2023, 2025; Fu et al., 2025; Chen et al., 2024b) or apply reinforcement learning for environment-aligned planning (Bai et al., 2025; Yang et al., 2024b; Qi et al., 2024; Feng et al., 2024; Zhou et al., 2024c; Wang et al., 2025), but suffer from high computational costs and poor generalization to unseen environments. Training-free methods build multi-agent frameworks for task decomposition and experience accumulation (Chen et al., 2024a; He et al., 2024; Sun et al., 2024; Yang et al., 2023b; Zhou et al., 2024b), yet their static pipelines and prompt-injected experience often fail to capture environment dynamics, yielding insufficient agent-environment alignment.

3 Method

3.1 Problem Formulation

Environment and Agent. In interactive decision tasks, we define the environment $\mathcal{E}$ as a tuple $(\mathcal{S}, \mathcal{A}, T, F, \mathcal{I})$, where $\mathcal{S}$ denotes the set of all possible states of the environment; $\mathcal{A}$ denotes the set of actions the agent can invoke; $T : \mathcal{S} \times \mathcal{A} \to \mathcal{S}$ defines how the environment state evolves in response to agent actions; $F : \mathcal{S} \times \mathcal{A} \to \mathcal{O}$ provides textual feedback that reflects the consequences of the action in the current state, where $\mathcal{O}$ is all possible observations; $\mathcal{I}$ encodes the *environment foundational information description*, a fixed, declarative representation of the environment's basic introduction, which is exposed to the agent at initialization. An agent π interacts with environment $\mathcal{E}$ by receiving task description and observations, then producing actions $a_t \in \mathcal{A}$. The interaction generates trajectory $\tau = [(s_0, a_0, o_0), \ldots, (s_T, a_T, o_T)]$, culminating in task completion feedback.

Formal Definition of Interface. Existing works typically assume the agent interacts directly with $\mathcal{E}$. However, we argue that this interaction is mediated by an **Interface**, denoted as Φ, which acts as a translation layer between the agent's cognitive space and the environment's execution space. Formally, we define the interface as a tuple of mapping functions: $\Phi = \langle f_{\text{info}}, f_{\text{act}}, f_{\text{obs}} \rangle$where each component serves a distinct role:

- **Information Augmenter** $f_{\text{info}} : \mathcal{I} \to \tilde{\mathcal{I}}$ exposes implicit environment logic (e.g., admissible action sequences) into an explicit descriptive context $\tilde{\mathcal{I}}$ provided at agent initialization.
- **Action Transducer** $f_{\text{act}} : \mathcal{A}_{\text{agent}} \to \mathcal{A}_{\text{env}} \cup \{\perp\}$ maps the agent's output to an executable environment command. If the output cannot be parsed, it returns an invalid symbol $\perp$.
- **Observation Transducer** $f_{\text{obs}} : \mathcal{S} \times \mathcal{A}_{\text{env}} \times \mathcal{O}_{\text{raw}} \to \mathcal{O}_{\text{agent}}$ transforms the raw feedback $\mathcal{O}_{\text{raw}}$ (from F) into an informative observation $\mathcal{O}_{\text{agent}}$ that better conveys the actual state transitions and their causes.

At each timestep t, the agent receives $\tilde{o}_t \in \mathcal{O}_{\text{agent}}$ (processed by f_{obs}) and generates $a_t \in \mathcal{A}_{\text{agent}}$, which is then executed as $a_t^{\text{env}} = f_{\text{act}}(a_t) \in \mathcal{A}_{\text{env}}$.

Agent-Environment Misalignment. We analyze the misalignment problem through the lens of the interface Φ. Ideally, Φ should be *lossless*, maximizing the mutual information between the agent's belief state and the ground-truth environment state. However, manually designed interfaces often exhibit **Semantic Gaps** through two mechanisms: (1) *state aliasing*, where a lossy f_{obs} maps distinct error states (e.g., wrong location vs. missing object) to the same generic observation (e.g., "Nothing happens."), preventing the agent from diagnosing failures; and (2) *under-specified constraints*, where critical preconditions of T (e.g., "open" requires "`go to`" first) are not encoded in $\tilde{\mathcal{I}}$ by f_{info}, leaving the agent under a hallucinated world model.

Therefore, we define **Agent-Environment Misalignment** as the discrepancy between the agent's expected state transition $s_{t+1}^{\text{expected}}$ (derived from its internal world model based on $\tilde{\mathcal{I}}$ and prior observations $[\tilde{o_0}, \tilde{o_1}, \ldots, \tilde{o_{t+1}}]$) and the actual transition $s_{t+1}^{\text{actual}} = T(s_t, a_t^{\text{env}})$, caused by insufficient expressiveness of the interface Φ.

Scope of This Work. We observe that misalignment in existing benchmarks primarily stems from information loss in f_{info} and f_{obs} rather than action space incompatibility. ALIGN therefore treats f_{act} as the identity mapping and focuses on automatically optimizing the other two components.

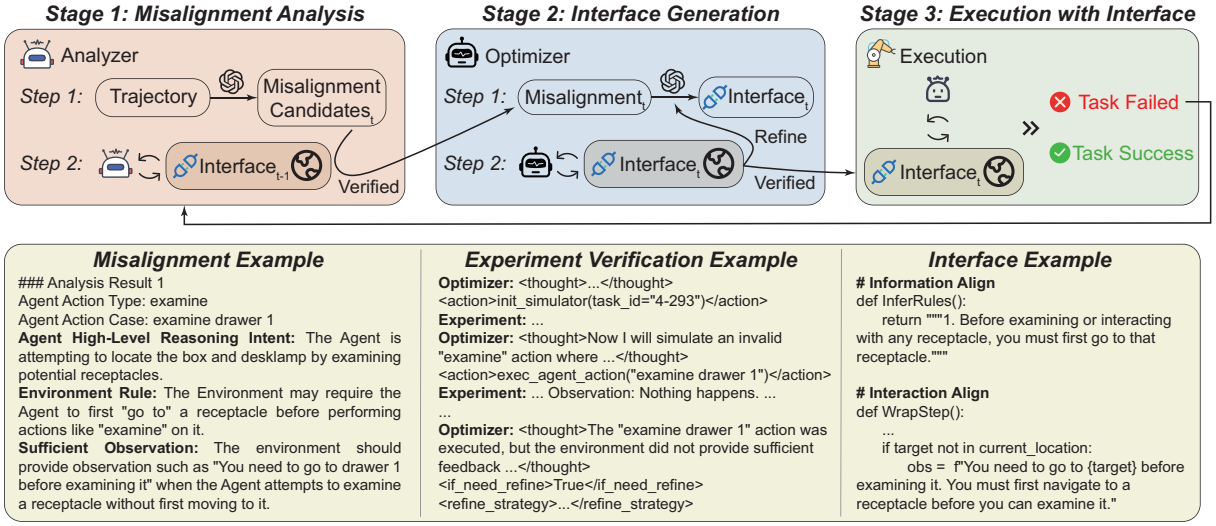

Figure 2: **ALIGN framework.** In each iteration, ALIGN progresses though three stages. **Stage 1**: the Analyzer identifies potential agent-environment misalignments and validates them through experiments; **Stage 2**: the Optimizer generates a new interface based on the previous interface and identified misalignments, followed by verification and refinement; **Stage 3**: the agent interacts with the updated interface-wrapped environment, with trajectories of failed tasks fed back to the Analyzer for analysis in the next iteration. At the bottom of the figure, examples for misalignment, verification of interface by Optimizer, and the ALIGN-generated interface are provided.

3.2 ALIGN Overview

We introduce **ALIGN** (Auto-Aligned Interface Generation), a framework that automatically generates an optimized interface Φ^* to bridge the semantic gaps identified in Section 3.1. As illustrated in Figure 3, ALIGN instantiates f_{info} and f_{obs} as two learnable modules implemented as a lightweight Python wrapper:

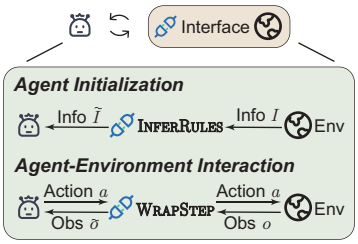

Figure 3: Overview of the ALIGN-generated interface. InferRules enriches static information ($\mathcal{I} \to \tilde{\mathcal{I}}$) at agent initialization, while WrapStep augments step-wise observations ($F \to \tilde{F}$) during interaction.

Interface Instantiation. As illustrated in Figure 3, ALIGN instantiates the theoretical interface components through two learnable modules implemented as a lightweight Python wrapper, without modifying the environment code or agent logic.

InferRules (implements f_{info}) extracts interaction rules and constraints from $(\text{task}, o_0, \mathcal{I})$ to produce $\tilde{\mathcal{I}}$, exposing precondition dependencies and action ordering requirements at initialization.

WrapStep (implements f_{obs}) intercepts F and augments each raw observation with diagnostic information to resolve state aliasing in interaction.

Together, these modules wrap $\mathcal{E}$ into an *augmented environment* $\tilde{\mathcal{E}} = (\mathcal{S}, \mathcal{A}, T, \tilde{F}, \mathcal{I} \cup \tilde{\mathcal{I}})$ with $\tilde{F}(s_t, a_t) := \text{WrapStep}(F, s_t, a_t)$, leaving the agent logic, the environment code, and the transition dynamics T unchanged. We denote the interface as $\Phi := \{\text{InferRules}, \text{WrapStep}\}$ in the remainder of this paper.

As shown in Figure 2, the ALIGN integrates two cooperative modules, **Analyzer** and **Optimizer**, to generate aligned interfaces. The framework operates through iterative optimization, with each iteration comprising three stages: in Stage 1, the Analyzer identifies agent-environment misalignments by analyzing past interaction trajectories; in Stage 2, the Optimizer generates, validates and refines a new interface based on the detected misalignments; and in Stage 3, the agent interacts with the environment wrapped with the newly generated interface, and the failed task trajectories are fed back to Analyzer for analysis in the next iteration.

3.3 ALIGN Framework

To automate the generation of interfaces that bridge the agent-environment misalignments, ALIGN need to solve two key challenges: (1) how to analyze and identify existing agent-environment misalignments, and (2) how to generate an interface

that addresses these misalignments. The overall algorithm process of ALIGN is outlined in Algorithm 1 in Appendix B.

Misalignment Analysis. We represent each agent-environment misalignment using structured text, as shown in the bottom left of Figure 2. The "Agent High-Level Reasoning Intent" and "Environment Rule" respectively depict the agent's expectations of the action and the environment's observation rules, together representing a misalignment. The "Sufficient Observation" represents the observation the environment should provide to resolve the misalignment. To analyze and identify these misalignments, we designed the Analyzer module based on LLMs. In each iteration, the Analyzer takes the failed interaction trajectory $\tau^{(i-1)}$ in the previous iteration, the set of currently identified misalignments $\mathcal{M}$, and the interface $\Phi^{(i-1)}$ from the previous round as input, and generates a new set of misalignments $\mathcal{M}^{(i)}$. Detailed prompts for this process are provided in Appendix E.4.

Interface Generation. Once the new set of misalignments $\mathcal{M}^{(i)}$ is identified, we employ the Optimizer module to generate a new interface. We represent the two modules of the interface, INFER-RULES and WRAPSTEP, as Python functions, as shown in the bottom right of Figure 2, to leverage the powerful code generation capabilities of LLMs. In each iteration, the Optimizer takes the newly identified misalignments $\mathcal{M}^{(i)}$ and the previous interface $\Phi^{(i-1)}$ as input, and generates a new interface $\Phi^{(i)}$. The detailed prompts for this process are provided in Appendix E.4.

Experimental Verification. Given the hallucination (Bang et al., 2023; Xu et al., 2024) issues of LLMs, we incorporate an experimental verification procedure. Specifically, after the Analyzer generates $\mathcal{M}^{(i)}$, it will interact with the environment wrapped by the previous interface $\Phi^{(i-1)}$ to validate whether the identified misalignments do indeed exist and can be resolved by the proposed "Sufficient Observation". And after the Optimizer generates the new interface $\Phi^{(i)}$, it will interact with the environment wrapped by this new interface to ensure that the generated interface can resolve the identified misalignments. If the Optimizer finds that the proposed interface is insufficient to address the discovered misalignments, it will provide a refinement strategy and regenerate the interface. This iterative process continues until the interface passes the validation, ensuring that the misalignments identified are appropriately addressed. An example of this process is provided in the bottom center of Figure 2. To facilitate this interaction with the interface-wrapped environment, we designed a set of encapsulated tools for both the Analyzer and Optimizer to use, as described in Appendix E.3.

After each iteration, the agent interacts with the environment wrapped by the new generated interface $\Phi^{(i)}$, and trajectories of the failed tasks are returned to Analyzer for further analysis. The algorithm continues iteratively until one of the following holds: (1) the pre-defined maximum number of iterations is reached; (2) no failed trajectories are produced; (3) no new misalignments are identified.

4 Experiment

4.1 Experimental Settings

Evaluation Protocol. We evaluate each agent in the original environment, then re-evaluate it in the same environment wrapped with ALIGN-generated interface. Interfaces are generated only from training tasks and held fixed during testing.

Benchmarks. We use ALFWorld (Shridhar et al., 2021) for embodied household tasks, ScienceWorld (Wang et al., 2022) for interactive scientific reasoning, WebShop (Yao et al., 2022) for web navigation, and M^{3}ToolEval (Wang et al., 2024b) for multi-turn tool use.

Agent Methods. We evaluate Vanilla Agent (no specialized prompting), ReAct (Yao et al., 2023) (interleaved reasoning and acting), Self-Consistency (Wang et al., 2023) (majority voting over sampled trajectories), Self-Refine (Madaan et al., 2023) (iterative self-critique) and Planning agent inspired by RAP (Hao et al., 2023) that decomposes tasks into sub-tasks.

Implementation Details. Unless otherwise noted, agents use Qwen2.5-7B-Instruct (Team, 2024) as the base model. Within ALIGN, the Optimizer uses Gemini 2.5 Pro (Google, 2025) for interface code generation, and GPT-4.1 (OpenAI, 2025) is used elsewhere in the Analyzer and Optimizer. Full setup is in Appendix E.

4.2 Main Results

Table 1 summarizes the task success rates or scores of five representative agent methods in the environment without (w/o) or with (w/) ALIGN-generated interface. The token consumption analysis can be found in Appendix D. Our empirical investigation yields three principal findings:

Method	Interface	Embodied		Web	Tool-use
		ALFWorld	ScienceWorld	WebShop	M^3ToolEval
Vanilla	w/o ALIGN	13.43	14.94	54.10	11.11
	w/ ALIGN	60.45 (+47.02)	27.69 (+12.75)	61.23 (+7.13)	20.83 (+9.72)
ReAct	w/o ALIGN	19.40	20.03	37.20	9.72
	w/ ALIGN	63.43 (+44.03)	28.97 (+8.94)	42.93 (+5.73)	18.06 (+8.34)
Self-Consistency	w/o ALIGN	11.94	14.07	56.23	11.11
	w/ ALIGN	69.40 (+57.46)	25.41 (+11.34)	61.10 (+4.87)	16.67 (+5.56)
Self-Refine	w/o ALIGN	3.73	14.87	44.80	5.55
	w/ ALIGN	40.30 (+36.57)	22.99 (+8.12)	52.30 (+7.50)	6.94 (+1.39)
Planning	w/o ALIGN	9.70	17.13	46.95	11.11
	w/ ALIGN	52.99 (+43.29)	26.34 (+9.21)	54.67 (+7.72)	18.06 (+6.95)

Table 1: **Effect of ALIGN-generated interfaces on four benchmarks.** For every agent we report its score without the interface (w/o ALIGN) and with the interface (w/ ALIGN); the value in parentheses is the absolute improvement. Metrics are task-success rate (%) for ALFWorld and M^3ToolEval, and scores for ScienceWorld and WebShop.

(1) ALIGN consistently enhances performance across different domains. All evaluated agent methods demonstrate significant performance improvements when utilizing ALIGN-generated interfaces. Specifically, the five agent methods exhibit mean improvements of 45.67% in task-success rate for ALFWorld, 10.07 points for ScienceWorld, 6.59 points for WebShop, and 6.39% in task-success rate for M^3ToolEval.

(2) Agent-environment misalignment is a pervasive phenomenon impeding the agent performance. The observed performance enhancements provide empirical evidence that numerous errors in baseline configurations originate from implicit constraints or under-specified observation, rather than from intrinsic reasoning deficiencies. This finding suggests that when these environmental constraints are explicitly surfaced, agents can execute their intended tasks with substantially improved reliability. Consequently, we posit that agent-environment misalignment is pervasive in interactive decision-making tasks, and addressing this problem is crucial for advancing agent performance.

(3) Alignment between agent and environment can facilitate identification of additional performance-influencing factors. While the Self-Consistency agent achieves a 69.40% success rate in ALFWorld with ALIGN, the performance of Self-Refine agent remains comparatively suboptimal (40.30%), indicating potential deficiencies in the critic and self-refinement capabilities of the Qwen2.5-7B-Instruct model. These limitations are similarly manifested in the M^3ToolEval results. Furthermore, the relatively modest performance improvements in ScienceWorld suggest that Qwen2.5-7B-Instruct may exhibit insufficient scientific causal reasoning capabilities. These observations indicate that properly aligning agent and environment enables more precise isolation and analysis of other factors influencing agent performance beyond alignment considerations.

4.3 Interface Quality Analysis

Influence on Agent Decision To quantitatively assess the influence of ALIGN-generated interfaces on agent decision beyond end-task performance metric, we introduce a metric that measures the frequency of *consecutive invalid actions* by calculating the proportion of the actions that occur within sequences of two or more consecutive `invalid` steps. Lower values of this metric indicate: (1) enhanced agent awareness of implicit preconditions, and (2) improved recovery capability following isolated errors. Table 2 presents the results for five agent methods implemented on ALFWorld and ScienceWorld. The empirical results demonstrate a substantial reduction in consecutive invalid actions frequency across all agent methods when utilizing ALIGN-generated interfaces. Specifically, we observe a mean reduction of 65% in ALFWorld and 49% in ScienceWorld. These findings provide evidence that ALIGN effectively enriches the information conveyed by the observation, preventing agents from entering repetitive error cycles, which aligns with the findings documented in Section 4.2.

Comparison with Agentic Systems and Human-designed Interfaces To further assess the effectiveness of our automatically generated interfaces, we compare ALIGN against (1) agentic frameworks equipped with carefully designed

Method	ALFWorld			ScienceWorld		
	w/o ALIGN	w/ ALIGN	Δ	w/o ALIGN	w/ ALIGN	Δ
Vanilla	77.91	26.59	66%	49.12	24.47	50%
ReAct	82.23	38.63	53%	46.61	29.99	36%
Self-Consistency	77.71	15.08	81%	51.10	31.51	38%
Self-Refine	90.38	45.84	49%	58.02	29.48	49%
Planning	74.09	19.14	74%	68.67	20.94	70%
Average	80.46	28.51	65%	54.70	27.28	49%

Table 2: **Impact of the ALIGN-generated interface on consecutive invalid actions.** The metric reports the fraction (%) of consecutive invalid actions. Lower values indicate more desirable behavior. Δ denotes the relative reduction with respect to the **w/o ALIGN** setting.

reasoning, planning and memory modules and (2) human-designed interfaces. The experimental setup and results are presented in Appendix C.2. As shown in Table 7, even without bespoke reasoning, planning, or memory modules, a vanilla agent that directly outputs the next action yields a 6.71 percentage points higher success rate than the best agentic system when paired with ALIGN-generated interfaces, indicating agent-environment misalignment substantially constrains the performance of LLM-based agents in interactive tasks. Moreover, using interfaces automatically generated by ALIGN yields a 13.44 percentage points higher than human-designed interfaces, further validating the effectiveness of our method (Table 8).

4.4 Generalization and Generality Study

Generalization Study To evaluate the generalization capabilities of ALIGN, we performed the following two experiments, with the results presented in Table 3 and detailed in Appendix C.3.

(a) Interface source: Vanilla agent				
Target method	ALF.	Sci.	Web.	M^3T.
ReAct	+39.56	+12.29	+7.87	+5.56
Self-Consistency	+51.49	+15.30	+3.00	+8.33
Self-Refine	+34.33	+14.11	+6.17	+4.17
Planning	+41.05	+9.66	+3.26	+11.11
(b) Interface source: Qwen2.5-7B-Instruct agent				
Target LLM	ALF.	Sci.	Web.	M^3T.
Qwen2.5-14B-Instruct	+17.46	+4.61	+4.66	+6.11
Llama3.1-8B-Instruct	+5.97	+10.27	+0.33	+0.83
Llama3.3-70B-Instruct	+5.82	+3.99	+5.68	+1.67

Table 3: **Generalization of ALIGN-generated interfaces across agents and models.** Mean performance improvements from applying ALIGN-generated interfaces in the four environments across different settings. (a) Cross-agent transfer: interfaces generated with a Vanilla agent improve other agent methods. (b) Cross-model transfer: interfaces generated with Qwen2.5-7B-Instruct can generalize to other LLMs.

(1) ALIGN can generalize to different agent architectures. Panel (a) of Table 3 applies interfaces generated with the Vanilla agent to the other four agents. Across all four environments every target agent shows consistent growth, demonstrating that ALIGN captures genuine and previously unexposed environment constraints. This also reinforces the earlier conclusion that agent-environment misalignment is a pervasive source of error independent of the agent's reasoning style.

(2) ALIGN can generalize to larger and heterogeneous LLMs. Panel (b) of Table 3 examines whether an interface generated with Qwen2.5-7B-Instruct can extend to larger or architecturally different model backbones. The results demonstrate that ALIGN-generated interfaces lead to performance improvements across base models of varying sizes and architectural families, which indicates that our method possesses strong generalization capabilities. We also observe that this generalization is not uniformly robust across all model families and datasets. For instance, Llama3.1-8B-Instruct (Meta, 2025a) shows only a marginal gain of +0.33 on the WebShop benchmark. This limited improvement may be attributed to the inherent reasoning capabilities of the model itself.

Taken together, these results show that ALIGN-generated interfaces can generalize (1) across agent policies and (2) across model scales and families, validating the practicality of ALIGN.

Generality Study In this work, our empirical observations indicate that the root cause of agent-environment misalignment lies in the robustness of the interface itself, making it a universal issue that affects agents irrespective of the underlying model capability. To further validate this claim and assess the generality of ALIGN, we conduct experiments on both closed-source LLMs and domain-specific models trained within the environment. For the former, we use the GPT-4.1 se-

(a) GPT-4.1 series		
Base Model	Interface	SR (%)
GPT-4.1-mini	w/o ALIGN	28.36
	w/ ALIGN	64.93 (+36.57)
GPT-4.1	w/o ALIGN	73.88
	w/ ALIGN	93.28 (+19.40)
(b) GiGPO-Qwen2.5-7B-Instruct		
Agent Method	Interface	SR (%)
Vanilla	w/o ALIGN	35.04
	w/ ALIGN	55.97 (+20.93)
Training Config	w/o ALIGN	89.55
	w/ ALIGN	92.54 (+2.99)

Table 4: **Generality of ALIGN.** Task success rates (SR) without and with ALIGN-generated interfaces in ALFWorld across two settings. (a) Using GPT-4.1 series models as the base model; (b) Using GiGPO-Qwen2.5-7B-Instruct under different agent architectures.

ries; for the latter, we use GiGPO-Qwen2.5-7B-Instruct-ALFWorld (Feng et al., 2025), a state-of-the-art model specifically post-trained on ALFWorld via reinforcement learning. Detailed experimental setup and full results are provided in Appendix C.4. As the results reported in Panel (a) of Table 4 shown, applying the ALIGN-generated interface substantially improves the performance of the GPT-4.1-based agent from 73.88% to 93.28%. Meanwhile, as the results reported in Panel (b) of Table 4 shown, the ALIGN-generated interface also enhances the performance of the domain-specific model under both our Vanilla Agent setting and its original training configuration, from 35.04% to 55.97% and 89.55% to 92.54%, respectively. These findings demonstrate that the fundamental and pervasive nature of agent-environment misalignment stems from deficiencies in the environment's interface rather than solely from the reasoning limitations of any given model, and further corroborate the generality of our method across both frontier and domain-specialized models.

4.5 Ablation Study

Ablation on Interface Components Starting from the full ALIGN interface, we ablate INFERRULES and WRAPSTEP separately. As shown in Table 5, both ablations reduce performance: w/o INFERRULES averages -6.72 percentage points on ALFWorld and -2.05 on ScienceWorld, while removing WRAPSTEP yields a larger decline of -31.79 percentage points and -7.84, respectively. These decreases confirm that each interface component contributes meaningfully. Moreover, the much larger drop w/o WRAPSTEP shows the critical role of fine-grained and enriched observation during interaction. This also suggests that rich, LLM-friendly observation should be prioritized by future environment designers when constructing environments.

	w/o INFERRULES		w/o WRAPSTEP	
Method	ALF.	Sci.	ALF.	Sci.
Vanilla	-8.96	-3.35	-33.58	-4.72
ReAct	-5.22	-2.08	-17.91	-6.44
Self-Consistency	-1.49	-2.30	-37.27	-10.59
Self-Refine	-7.46	-1.72	-34.33	-7.59
Planning	-10.45	-0.78	-26.87	-9.86
Mean	-6.72	-2.05	-31.79	-7.84

Table 5: **Ablation on Interface components.** Values show performance change on ALFWorld and ScienceWorld. Negative values mean drops from *Full* interface.

Temp.	Iter0	Iter1	Iter2	Iter3
0.2	13.43	22.39	0.00	0.00
0.5	13.43	23.88	1.49	0.75

Table 6: Task success rate (%) on ALFWorld across iterations without experimental verification procedure.

Ablation on Experimental Verification To assess whether the experimental verification procedure in Section 3.3 is indispensable, we ablated it with the Vanilla agent on ALFWorld. As a surrogate, the Analyzer and Optimizer each sampled six candidates per iteration and selected their top one, under decoding temperatures $T \in \{0.2, 0.5\}$. As shown in Table 6, success rate deteriorates sharply across iterations, reflecting the limited single-shot reliability of LLMs in diagnosing misalignments and synthesizing interfaces, and confirming the necessity of experimental verification.

5 Conclusion

In this work, we introduce **ALIGN**, a framework that automatically generates aligned interfaces to alleviate the **agent-environment misalignment** in interactive decision-making tasks. By diagnosing implicit constraints via the Analyzer and synthesizing interfaces via the Optimizer, ALIGN achieves significant improvements across four benchmarks spanning embodied tasks, web navigation, and tool-use. Our results show that ALIGN generalizes to unseen models and strategies, offering a robust, plug-and-play solution that decouples agent design from manual environment-specific alignment.

Limitations

Despite the effectiveness of ALIGN in alleviating agent-environment misalignment, this work represents an initial exploration into automated interface generation. Several important directions remain open for further investigation:

Toward more diverse and complex environments. Our current evaluation focuses on environments with discrete, text-based action spaces across three domains: embodied tasks, web navigation, and tool-use. ALIGN's applicability to more complex settings remains to be explored. Future work could investigate more complex environments like extending ALIGN to multimodal domains such as GUI agents, where interfaces must process visual observations alongside textual feedback.

Metrics for interface quality. This paper evaluates interface effectiveness primarily through task success rates and consecutive invalid actions. More comprehensive metrics are needed to quantify interface influence on agent behavior. Promising directions include: (1) developing finer-grained behavioral diagnostics measuring specific aspects of agent understanding, such as exploratory actions or strategy diversity; (2) employing LLM-as-a-Judge (Zheng et al., 2023) paradigms to evaluate whether interfaces successfully convey environment constraints.

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A LLM Usage Statement

Throughout the completion of this work, the LLM was employed solely for the purpose of refining sentences and improving grammatical accuracy during the manuscript writing process.

B Formalization of the ALIGN Algorithm

The formalization of the ALIGN algorithm is outlined in Algorithm 1.

Algorithm 1 ALIGN: Auto-Aligned Interface Generation

Require: Environment $\mathcal{E}$, Agent π, Task training set $\mathcal{T}_{\text{train}}$, Maximum iterations K

Initialize misalignment set $\mathcal{M} \leftarrow \emptyset$, interface $\Phi^{(0)} \leftarrow \{\textsc{InferRules}^{(0)}, \textsc{WrapStep}^{(0)}\}$, where $\textsc{InferRules}^{(0)}$ and $\textsc{WrapStep}^{(0)}$ are identity functions
for $i = 1, 2, \ldots, K$ **do**
  $\tilde{\mathcal{E}}^{(i-1)} \leftarrow$ Environment $\mathcal{E}$ wrapped with interface $\Phi^{(i-1)}$
  $\tau_{\text{fail}}^{(i-1)} \leftarrow$ Failed trajectories from agent π interacting with $\tilde{\mathcal{E}}^{(i-1)}$ on $\mathcal{T}_{\text{train}}$
  if $\tau_{\text{fail}}^{(i-1)} = \emptyset$ **then**
    break ▷ No more failures in the training set
  end if
  // Stage 1: Misalignment Analysis
  $\mathcal{M}^{(i)} \leftarrow \text{Analyzer}(\tau_{\text{fail}}^{(i-1)}, \mathcal{M}, \Phi^{(i-1)})$
  if $\mathcal{M}^{(i)} = \emptyset$ **then**
    break ▷ No new misalignments identified
  end if
  $\mathcal{M} \leftarrow \mathcal{M} \cup \mathcal{M}^{(i)}$
  // Stage 2: Interface Generation
  $\Phi^{(i)} \leftarrow \text{Optimizer}(\mathcal{M}^{(i)}, \Phi^{(i-1)})$
end for
return final interface $\Phi^{(i)}$

C Supplementary Experimental Setup and Detailed Results

C.1 Preliminary Experiments

To preliminarily assess the significance of agent-environment misalignment, we conducted exploratory experiments on the ALFWorld. We employed the vanilla Qwen2.5-7B-Instruct agent with a temperature setting of 0.0. The deployment protocol, prompt template, followed the same configuration described in Appendix E and Appendix E.4.

During the experiments, we introduced a minor modification to the environment: if the agent issued the action *examine receptacle* and the environment returned the default observation "Nothing happens.", we replaced it with "You need to first go to receptacle before you can examine it." This simple adjustment increased the agent's task success rate from 13.4% to 31.3%.

C.2 Interface Quality Analysis Experiments

To further assess the quality of the ALIGN-generated interface, we first compare our method with human-designed agentic system. Our experiments are conducted on ALFWorld using the AgentSquare (Shang et al., 2025) framework. To maximize the advantages of the agentic system, we adopt gpt-4.1-2025-04-14 as the base model, select OPENAGI (Ge et al., 2023) for the planning module, Self-Refine (Madaan et al., 2023) for the reasoning module, and evaluate memory using Generative (Park et al., 2023), DiLu (Wen et al., 2024), TP (Yu et al., 2024), and VOYAGER (Wang et al., 2024a). For our approach, we employ a gpt-4.1-2025-04-14-based vanilla agent, where the interface is generated with the gpt-4.1-2025-04-14-mini-based vanilla agent by ALIGN (the experimental setup is same as Appendix C.4). The results are reported in Table 7.

Furthermore, we compare the ALIGN-generated interface against the human-designed interface. We adopt the following configurations for comparison with our method: (1) **Few-shot:** Settings identical to those in the ReAct (Yao et al., 2023); (2) **Valid Actions:** Supplying the agent with all valid actions at every response turn, analogous to the `check_valid_actions` configuration in AgentBoard (Ma et al., 2024); (3) **Human-Designed Interface:** Interfaces manually crafted by Ph.D. students after inspecting ALFWorld experiments, examining trajectories, and running experiments themselves. The design logic includes: executing "go to" prior to each action; automatically checking object labels; converting "put" to "move" when appropriate; returning the action space upon invalid actions; issuing reminders when "clean with" is applied to non-sinkbasin objects; and other hand-engineered rules. We use Qwen2.5-7B-Instruct as the base model. Experimental results are reported in Table 8.

C.3 Generalization Study Experiments

Detailed results of the generalization study are provided for the cross-method experiments in Table 9 and for the cross-model experiments in Tables 10, 11, and 12.

C.4 Generality Study Experiments

For the validation on closed-source LLMs, we selected the GPT-4.1 family. Specifically, we experimented with gpt-4.1-mini-2025-04-14 and gpt-4.1-

Agent Framework	Interface	Memory Module	pick and place	pick clean and place	pick heat and place	pick cool and place	look at / examine in light	pick two obj and place	Success Rate (%)
AgentSquare	/	Generative	95.83	87.10	69.57	95.24	83.33	88.24	86.57
AgentSquare	/	DiLu	91.67	87.10	52.17	95.24	83.33	70.59	80.60
AgentSquare	/	TP	87.50	51.61	4.35	61.90	27.78	47.06	47.76
AgentSquare	/	VOYAGER	95.83	83.87	52.17	90.48	83.33	64.71	79.10
Vanilla Agent	w/o ALIGN	/	100.00	93.55	13.04	71.43	61.11	100.00	73.88
Vanilla Agent	w/ ALIGN	/	100.00	100.00	78.26	100.00	77.78	100.00	**93.28**

Table 7: Experimental results of the comparison between agents with ALIGN-generated interface and agents with human-designed reasoning, planning and memory module.

Experimental Setting	Success Rate (%)
w/o Interface	13.43
Few-shot	44.78
Valid Actions	44.03
Human Designed Interface	47.01
ALIGN-generated Interface	**60.45**

Table 8: Experimental results of the comparison between agents with ALIGN-generated interface and agents with human-designed interfaces.

2025-04-14. First, we used gpt-4.1-mini-2025-04-14 as the base model to instantiate a Vanilla Agent and synthesize interface with ALIGN. We then applied the same interface to an agent powered by gpt-4.1-2025-04-14. All other experimental settings were identical to those in the main experiments. The results are presented in Table 13.

For domain-specific models trained within the environment, we used GiGPO-Qwen2.5-7B-Instruct-ALFWorld, a state-of-the-art model post-trained on ALFWorld via reinforcement learning (Feng et al., 2025). We reused the interface produced in our main experiment (generated with the base Qwen2.5-7B-Instruct model under the Vanilla Agent method). At evaluation time, we considered two configurations: (1) our Vanilla Agent setting, and (2) a configuration that matches the logic and prompt setting used during training in the original paper.

C.5 Ablation Study Experiments

The full result of interface ablation experiment can be found in Table 14.

D Token Consumption Analysis

The average token consumption per iteration in the main experiment described in Section 4.1 is shown in Table 15.

Due to the "Experimental Verification" setup, the Analyzer and Optimizer need to interact with the environment multiple times, and all previous interaction histories are included as new prompt inputs to the LLM in each round of interaction. Additionally, when the Optimizer identifies that the generated interface is imperfect, it needs to refine the previously generated interface and conduct experimental verification again, leading to increased token consumption. However, as LLM capabilities continue to improve and hallucination issues decrease, this cost will gradually reduce. Furthermore, it is worth noting that:

- The INFERRULES wrapper and WRAPSTEP wrapper are implemented as python logic code, which does not involve calls to models or agents, therefore not incurring additional token consumption. On the contrary, as demonstrated in our experiments in Section 4.3, **using ALIGN-generated interfaces can help agents reduce repetitive meaningless actions, thereby reducing the number of LLM calls and decreasing token consumption** compared to not using ALIGN-generated interfaces.
- Except when the Optimizer generates interface codes requiring the cutting edge LLMs (such as Gemini 2.5 Pro), weaker and more cost-effective LLMs (such as GPT-4.1-mini) can be used at other times, which will significantly reduce the operational costs of ALIGN.
- ALIGN-generated interfaces can generalize to different agent architectures and base LLMs. This means that for each environment, using the ALIGN method to generate an interface only once can bring performance improvements to different agents, regardless of agent

Base Method: Vanilla		Embodied		Web	Tool-use
Method	**Interface**	**ALFWorld**	**ScienceWorld**	**WebShop**	**M^3ToolEval**
ReAct	w/o ALIGN	19.40	20.03	37.20	9.72
	w/ ALIGN	58.96 (+39.56)	32.32 (+12.29)	45.07 (+7.87)	15.28 (+5.56)
Self-Consistency	w/o ALIGN	11.94	14.07	56.23	11.11
	w/ ALIGN	63.43 (+51.49)	29.37 (+15.30)	59.23 (+3.00)	19.44 (+8.33)
Self-Refine	w/o ALIGN	3.73	14.87	44.80	5.55
	w/ ALIGN	38.06 (+34.33)	28.98 (+14.11)	50.97 (+6.17)	9.72 (+4.17)
Planning	w/o ALIGN	9.70	17.13	46.95	11.11
	w/ ALIGN	50.75 (+41.05)	26.79 (+9.66)	50.21 (+3.26)	22.22 (+11.11)

Table 9: **Generalization of ALIGN-generated interfaces generated with Vanilla agents to other agent methods.** For each agent we report its score without the interface (w/o ALIGN) and with the interface (w/ ALIGN); the value in parentheses is the *absolute* improvement.

Base Model: Qwen2.5-14B-Instruct		Embodied		Web	Tool-use
Method	**Interface**	**ALFWorld**	**ScienceWorld**	**WebShop**	**M^3ToolEval**
Vanilla	w/o ALIGN	48.51	22.58	53.67	13.89
	w/ ALIGN	52.24 (+3.73)	37.58 (+15.00)	58.40 (+4.73)	18.06 (+4.17)
ReAct	w/o ALIGN	54.48	31.24	39.73	15.28
	w/ ALIGN	70.15 (+15.67)	29.79 (-1.45)	42.17 (+2.44)	26.39 (+11.11)
Self-Consistency	w/o ALIGN	43.28	25.60	52.63	13.89
	w/ ALIGN	72.39 (+29.11)	26.68 (+1.08)	51.07 (-1.56)	27.78 (+13.89)
Self-Refine	w/o ALIGN	5.22	18.97	41.00	15.28
	w/ ALIGN	14.18 (+8.96)	20.72 (+1.75)	39.93 (-1.07)	16.67 (+1.39)
Planning	w/o ALIGN	49.25	21.46	31.72	25.00
	w/ ALIGN	79.10 (+29.85)	28.13 (+6.67)	50.47 (+18.75)	25.00 (0.00)

Table 10: **Generalization of ALIGN-generated interfaces generated with Qwen2.5-7B-Instruct to Qwen2.5-14B-Instruct.** For each agent we report its score without the interface (w/o ALIGN) and with the interface (w/ ALIGN); the value in parentheses is the *absolute* improvement.

Base Model: Llama3.1-8B-Instruct		Embodied		Web	Tool-use
Method	**Interface**	**ALFWorld**	**ScienceWorld**	**WebShop**	**M^3ToolEval**
Vanilla	w/o ALIGN	5.22	23.59	35.17	5.56
	w/ ALIGN	14.18 (+8.96)	36.40 (+12.81)	24.00 (-11.17)	1.39 (-4.17)
ReAct	w/o ALIGN	1.49	22.42	27.12	12.50
	w/ ALIGN	15.67 (+14.18)	28.74 (+6.32)	27.10 (-0.02)	22.22 (+9.72)
Self-Consistency	w/o ALIGN	5.22	25.21	29.80	4.17
	w/ ALIGN	11.94 (+6.72)	34.83 (+9.62)	15.83 (-13.97)	2.78 (-1.39)
Self-Refine	w/o ALIGN	0.00	22.34	27.70	1.39
	w/ ALIGN	0.75 (+0.75)	31.33 (+8.99)	37.43 (+9.73)	1.39 (0.00)
Planning	w/o ALIGN	6.72	13.33	23.67	4.17
	w/ ALIGN	5.97 (-0.75)	26.95 (+13.62)	40.77 (+17.10)	4.17 (0.00)

Table 11: **Generalization of ALIGN-generated interfaces generated with Qwen2.5-7B-Instruct to Llama3.1-8B-Instruct.** For each agent we report its score without the interface (w/o ALIGN) and with the interface (w/ ALIGN); the value in parentheses is the *absolute* improvement.

Base Model: Llama3.3-70B-Instruct		Embodied		Web	Tool-use
Method	**Interface**	**ALFWorld**	**ScienceWorld**	**WebShop**	**M^{3}ToolEval**
Vanilla	w/o ALIGN	52.99	55.77	51.67	37.50
	w/ ALIGN	43.28 (-9.71)	57.74 (+1.97)	62.07 (+10.40)	33.33 (-4.17)
ReAct	w/o ALIGN	45.52	56.50	58.22	34.72
	w/ ALIGN	47.01 (+1.49)	58.28 (+1.78)	53.83 (-4.39)	43.06 (+8.34)
Self-Consistency	w/o ALIGN	54.48	56.66	50.37	36.11
	w/ ALIGN	65.67 (+11.19)	59.24 (+2.58)	55.63 (+5.26)	34.72 (-1.39)
Self-Refine	w/o ALIGN	38.06	56.97	38.40	1.39
	w/ ALIGN	46.27 (+8.21)	60.17 (+3.20)	47.85 (+9.45)	0.00 (-1.39)
Planning	w/o ALIGN	58.96	48.75	54.90	33.33
	w/ ALIGN	76.87 (+17.91)	59.17 (+10.42)	62.60 (+7.70)	40.28 (+6.95)

Table 12: **Generalization of ALIGN-generated interfaces generated with Qwen2.5-7B-Instruct to Llama3.3-70B-Instruct.** For each agent we report its score without the interface (w/o ALIGN) and with the interface (w/ ALIGN); the value in parentheses is the *absolute* improvement.

Base Model	Interface	pick and place	pick clean and place	pick heat and place	pick cool and place	look at / examine in light	pick two obj and place	Success Rate (%)
gpt-4.1-mini	w/o ALIGN	58.33	22.58	8.70	9.52	22.22	52.94	28.36
	w/ ALIGN	95.83	87.10	26.09	80.95	27.78	52.94	**64.93**
gpt-4.1	w/o ALIGN	100.00	93.55	13.04	71.43	61.11	100.00	73.88
	w/ ALIGN	100.00	100.00	78.26	100.00	77.78	100.00	**93.28**

Table 13: Experimental results for GPT-4.1 series agents with ALIGN on ALFWorld.

Method	Interface	Embodied		Web	Tool
		ALFWorld	**ScienceWorld**	**Webshop**	**M^{3}ToolEval**
Vanilla	Full	60.45	27.69	61.23	20.83
	w/o INFERRULES	51.49 (-8.96)	24.34 (-3.35)	51.03 (-10.20)	18.06 (-2.77)
	w/o WRAPSTEP	26.87 (-33.58)	22.97 (-4.72)	61.23 (-0.00)	11.11 (-9.72)
ReAct	Full	63.43	28.97	42.93	18.06
	w/o INFERRULES	58.21 (-5.22)	26.89 (-2.08)	35.97 (-6.96)	9.72 (-8.34)
	w/o WRAPSTEP	45.52 (-17.91)	22.53 (-6.44)	47.60 (+4.67)	19.44 (+1.38)
Self-Consistency	Full	69.40	25.41	61.10	16.67
	w/o INFERRULES	67.91 (-1.49)	23.11 (-2.30)	55.67 (-5.43)	13.89 (-2.78)
	w/o WRAPSTEP	23.13 (-17.91)	14.82 (-10.59)	60.67 (-0.43)	15.28 (-1.39)
Self-Refine	Full	40.30	22.99	52.30	6.94
	w/o INFERRULES	32.84 (-7.46)	21.27 (-1.72)	46.33 (-5.97)	6.94 (-0.00)
	w/o WRAPSTEP	5.97 (-34.33)	15.40 (-7.59)	47.80 (-4.50)	6.94 (-0.00)
Planning	Full	52.99	26.34	54.67	18.06
	w/o INFERRULES	42.54 (-10.45)	25.56 (-0.78)	48.18 (-6.49)	16.67 (-1.39)
	w/o WRAPSTEP	26.12 (-26.87)	16.48 (-9.86)	52.87 (-1.80)	16.67 (-1.39)

Table 14: Ablation study on the components of ALIGN. Values represent task success rates (%) or scores. For ablated conditions (w/o INFERRULES, w/o WRAPSTEP), performance changes from the 'Full' are shown in parentheses.

		ALFWorld	ScienceWorld	WebShop	M^{3}ToolEval
Analyzer	Input Token (M)	0.2770	0.4333	0.1783	0.1094
	Output Token (M)	0.0040	0.0036	0.0048	0.0016
	Total Token (M)	0.2809	0.4370	0.1831	0.1109
Optimizer	Input Token (M)	0.2619	0.2288	0.0669	0.1100
	Output Token (M)	0.0087	0.0172	0.0040	0.0118
	Total Token (M)	0.2706	0.2460	0.0709	0.1217
Total	Total Token (M)	0.5515	0.6830	0.2540	0.2326

Table 15: The average token consumption per iteration in the main experiment described in Section 4.1.

version updates. This also means that **the cost of interface generation is a one-time expense**, rather than requiring the generation of new interfaces for each task execution. Therefore, from an amortization perspective, the method's cost becomes increasingly economical as the environment is utilized more frequently, with the one-time interface design cost being distributed across multiple uses and becoming proportionally smaller with increased usage.

E Implementation Details

E.1 Benchmarks Task Splits

The task splits of benchmarks we use are as follows:

(1) ALFWorld (Shridhar et al., 2021): We adhere to the original dataset partitioning presented in the paper, wherein the tasks from the "eval_out_of_distribution" category are used as the test set, and the "train" category is designated as the training set. In each iteration, we randomly select three tasks from the training set of each task type to serve as the training data for the agent's interaction.

(2) ScienceWorld (Wang et al., 2022):We follow the original partitioning of the train and test sets as described in the paper. For efficiency reasons, during testing, we select at most the first five tasks from the 30 available task types for evaluation. In each iteration, we randomly select one task from the training set of each task type to be used as the training data for the agent's interaction.

(3) WebShop (Yao et al., 2022): In alignment with the setup of Yao et al. (2023), we use tasks with IDs ranging from 0 to 49 (50 tasks in total) as the test set, and tasks with IDs from 50 to 199 (150 tasks in total) as the training set. In each iteration, we randomly select 20 tasks from the training set to serve as the training data for the agent's interaction.

(4) M^{3}ToolEval (Wang et al., 2024b): Since M^{3}ToolEval does not provide a distinct training set division, we select two tasks from each task type in the original dataset as the training set, with the remaining tasks used as the test set. In each iteration, the entire training set is utilized for the agent's interaction.

E.2 Hyperparameter and Experimental Setting

For all the agents, we deploy them uniformly using vllm (Kwon et al., 2023) across 8 Nvidia A100 80GB GPUs, with the inference temperature set to 0.0. The models utilized contain Qwen2.5-7B-Instruct[1] (Team, 2024), Qwen2.5-14B-Instruct[2] (Team, 2024), Llama3.1-8B-Instruct[3] (Meta, 2025a) and Llama3.3-70B-Instruct[4] (Meta, 2025b).

In ALIGN, we use Gemini 2.5 Pro (gemini-2.5-pro-exp-03-25)(Google, 2025) for Optimizer to generate new interface, with the temperature set to 0.2. For other scenarios requiring the use of an LLM, we employ GPT-4.1 (gpt-4.1-2025-04-14)(OpenAI, 2025). We set $K = 8$ during experiments.

E.3 Tools for Experimental Verification

In order to implement the experimental verification process mentioned in Section 3.3, we have encapsulated the following tools for Analyzer and Optimizer to interact with the interface-wrapped environment:

(1) `init_simulator(task_id, interface)`: Initializes an experimental task, specifying the task ID and the interface code.

[1]https://huggingface.co/Qwen/Qwen2.5-7B-Instruct
[2]https://huggingface.co/Qwen/Qwen2.5-14B-Instruct
[3]https://huggingface.co/meta-llama/Llama-3.1-8B-Instruct
[4]https://huggingface.co/meta-llama/Llama-3.3-70B-Instruct

(2) `reset_simulator()`: Resets the experimental task.

(3) `run_task()`: Runs the current task until completion, returning the interaction trajectory.

(4) `exec_agent_action(agent_action)`: Executes a specific action and returns the enhanced observation after the interface processing.

(5) `get_agent_action()`: Based on the current trajectory, returns the next action to be issued by the agent.

(6) `change_obs(obs)`: Modifies the observation of the previous action execution.

E.4 Prompt Templates

We present the prompt template of the Analyzer and Optimizer for ALFWorld. For the prompt templates of other benchmarks, please refer to the supplemental materials. For the WebShop and M^3ToolEval environments, no "Gold Action and Observation Sequence" is provided.

Analyzer Prompt Template of Misalignment Analysis

User message:
In modern benchmarks evaluating LLM Agent reasoning capabilities, human designers create an Environment with a set of rules defining how tasks are accomplished. These rules, referred to as the Environment's World Model, specify the sequence of actions required to achieve specific outcomes. For example, the Environment's World Model might dictate that certain actions (e.g., operating on a receptacle) can only be performed after prerequisite actions (e.g., moving to the receptacle).

Meanwhile, the Agent operates based on its own World Model, which it constructs by interpreting the task and environment prompts. The Agent first determines its high-level reasoning intent—its understanding of what needs to be done—and then selects actions according to its internal World Model. However, because the Environment's World Model is manually crafted and may not be fully conveyed through prompts, the Agent's World Model might differ, leading to unexpected behavior. For instance, the Agent might choose an action that aligns with its intent but violates the Environment's rules, or it might misinterpret feedback due to insufficient information from the Environment.

We define a misalignment between the Environment's World Model and the Agent's World Model as a situation where:
- The Environment provides feedback that does not sufficiently clarify its World Model, leaving the Agent unable to adjust its understanding of the rules.

Your task is to analyze the logs from a recent task to determine whether such a misalignment occurred, preventing a fair assessment of the Agent's capabilities. And this misalignment has not been fixed by current 'WrapStep' function. Your analysis will guide us in addressing this issue moving forward.

Experimental Environment Evaluation Template

```python
{{ experimental_template }}
```

In this template, the function 'InferRules' is used to define the environment rules. The function 'WrapStep' handles post-processing of the Agent's actions (e.g., splitting them into multiple steps, performing pre-checks, returning more detailed feedback, etc.). This function should not interfere with the Agent's own reasoning. There current implementation is as follows:

```python
{{ Interface }}
```

Environment Logs

```txt
{{ logs }}
```

Here, each ‘Observation‘ is the feedback returned to the Agent after it executes an action.

Gold Action and Observation Sequence

```txt
{{ gold_action_obs_sequence }}
```

Environment Logics and Misalignment Analyzed in the Previous Steps

{{ environment_logics }}

Your Task

Determine whether, during this task, there was a misalignment between the Environment’s World Model and the Agent’s World Model that hindered a fair assessment of the Agent’s capabilities. Choose exactly one of the following outputs:

If there is NO misalignment (i.e., the Agent’s failures stem from its own errors or limitations, not a mismatch with the Environment’s World Model), output:
<analysis_result> No Misalignment </analysis_result>

If there IS a misalignment (i.e., the Environment’s World Model conflicts with the Agent’s World Model), output:
<analysis_result> Found Misalignment </analysis_result>
<environment_logic_and_misalignments> the new environment rules and misalignments identified by you, which have not been fixed by current ‘WrapStep‘ function. </environment_logic_and_misalignments>

The format of the environment logic and misalignment is as follows:
```txt
### Analysis Result 1
Analysis Task ID: xxx
Agent Action Type: xxx # The type of action the Agent attempted to perform, such as "examine", "move object to receptacle", etc.
Agent Action Case: xxx # The specific action the Agent attempted to perform.
Agent High-Level Reasoning Intent: xxx # The Agent’s high-level reasoning intent, which may be a general description of the action it was trying to perform.
Environment World Model Rule: xxx # The rule from the Environment’s World Model that don’t align the Agent’s World Model.
Sufficient Environment Feedback: xxx # to offer the Agent adequate information to bridge gaps in understanding the environment’s world model. such as "The environment should provide ’xxx’ feedback when the Agent attempts to operate on a receptacle without first going to it."
Type: "Bug of current WrapStep function" or "Need to add new logic in the WrapStep function"

### Analysis Result 2
...
```

Note: You should not generate duplicate misalignment analysis results as the ones already provided in the ‘Environment Logics and Misalignment Analyzed in the Previous Steps‘ section.

Analyzer Prompt Template of Experimental Verification

User message:
Now you should conduct simulation experiments in the simulator to verify that

the environment rules you hypothesized and Misalignment you identified truly exists. You must perform sufficient experiments to confirm or refute your suspicion.

Here are the operations you can use:

1. init_simulator(task_id: str)
- Initializes a new simulator for the specified ‘task_id‘.
- ‘task_id‘ must be in the format ’int-int’ where the first int $\in$ [0, 5].
- The different task types are mapped as follows:

0: ’pick_and_place’,
1: ’pick_clean_and_place’,
2: ’pick_heat_and_place’,
3: ’pick_cool_and_place’,
4: ’look_at_or_examine_in_light’,
5: ’pick_two_obj_and_place’

- All subsequent operations occur within this initialized simulator.

2. reset_simulator()
- Resets the current simulator to its initial state.

3. execute_agent_action(agent_action: str)
- Executes an agent action using the ‘WrapStep‘ function.

4. change_last_action_observation(obs: str)
- Updates the last observation returned by the simulator to the specified ‘obs‘.
- This is useful for simulating the agent’s next action in a different environment feedback context.

5. get_next_agent_action()
- Retrieves the next action that the real Agent would perform under the current simulation conditions.
- Note: The Agent’s choice of the next action is based on the current environment state, including the outcomes of any previous ‘step()‘ or ‘get_next_agent_action()‘ call, along with the latest observations.

If you believe you have reached a conclusion from your experiments, provide it in this format:

<thought> Your reasoning here </thought>
<environment_logic_and_misalignments> the new environment rules and misalignments identified by you, which have not been fixed by current ‘WrapStep‘ function. </environment_logic_and_misalignments>

The format of the environment logic and misalignment is as follows:
“‘txt
Analysis Result 1
Analysis Task ID: xxx
Agent Action Type: xxx # The type of action the Agent attempted to perform, such as "examine", "move object to receptacle", etc.
Agent Action Case: xxx # The specific action the Agent attempted to perform.
Agent High-Level Reasoning Intent: xxx # The Agent’s high-level reasoning intent, which may be a general description of the action it was trying to perform.
Environment World Model Rule: xxx # The rule from the Environment’s World Model that don’t align the Agent’s World Model.
Sufficient Environment Feedback: xxx # to offer the Agent adequate information to bridge gaps in understanding the environment’s world model. such as "The environment should provide ’xxx’ feedback when the Agent attempts to operate on a receptacle without first going to it."
Type: "Bug of current WrapStep function" or "Need to add new logic in the WrapStep function"

Analysis Result 2
...
“‘

If you need to carry out more operations in the simulator, respond in the following format, specifying exactly one operation per turn:

<thought> Your reasoning here, you

should consider all hypotheses if the simulation result is not as expected </thought>
<action> The single operation you wish to perform (e.g., init_simulator(task_id="xy"), step(action="x"), execute_agent_action(agent_action="x"), etc.) </action>

Note:
You should verify the correctness of the following, step by step, through your experiments:
1. environment_rules: Use ‘execute_agent_action‘ to confirm that the environment rules you hypothesized are indeed correct, and current ‘WrapStep‘ function is not sufficient.
2. agent_intent_description: Obtain the Agent’s intended behavior (e.g., via ‘get_next_agent_action‘) and simulate it by using ‘WrapStep‘ to confirm whether it aligns with your description.
3. identified_misalignment: Through chaning the environment feedback, you can verify whether the misalignment you identified is indeed correct and the environment feedback you hypothesized is indeed sufficient. You can use ‘WrapStep‘ to simulate the agent’s action, then use ‘change_last_action_observation‘ to change the environment feedback, and finally use ‘get_next_agent_action‘ to check whether the agent can correctly identify the next action.

Analyzer Prompt Template of Reranking Misalignments Analysis (Ablation Study)

User message:
In modern benchmarks evaluating LLM Agent reasoning capabilities, human designers create an Environment with a set of rules defining how tasks are accomplished. These rules, referred to as the Environment’s World Model, specify the sequence of actions required to achieve specific outcomes. For example, the Environment’s World Model might dictate that certain actions (e.g., operating on a receptacle) can only be performed after prerequisite actions (e.g., moving to the receptacle).

Meanwhile, the Agent operates based on its own World Model, which it constructs by interpreting the task and environment prompts. The Agent first determines its high-level reasoning intent—its understanding of what needs to be done—and then selects actions according to its internal World Model. However, because the Environment’s World Model is manually crafted and may not be fully conveyed through prompts, the Agent’s World Model might differ, leading to unexpected behavior. For instance, the Agent might choose an action that aligns with its intent but violates the Environment’s rules, or it might misinterpret feedback due to insufficient information from the Environment.

We define a misalignment between the Environment’s World Model and the Agent’s World Model as a situation where:
- The Environment provides feedback that does not sufficiently clarify its World Model, leaving the Agent unable to adjust its understanding of the rules.

Now other human experts have analyzed the logs from a recent task and identified some potential misalignments. Your task is to review these misalignments and choose the most appropriate one.

Experimental Environment Evaluation Template

“‘python
{{ experimental_template }}
“‘

In this template, the function ‘Infer-Rules‘ is used to define the environment rules. The function ‘WrapStep‘ handles post-processing of the Agent’s actions

(e.g., splitting them into multiple steps, performing pre-checks, returning more detailed feedback, etc.). This function should not interfere with the Agent's own reasoning. There current implementation is as follows:

```python
{{ Interface }}
```

Environment Logs

```txt
{{ logs }}
```

Here, each 'Observation' is the feedback returned to the Agent after it executes an action.

Gold Action and Observation Sequence

```txt
{{ gold_action_obs_sequence }}
```

Environment Logics and Misalignment Analyzed in the Previous Steps

{{ environment_logics }} Note: These logics may not be accurate. They are the environment rules that were previously hypothesized and may contain errors.

Your Task

Choose the most appropriate misalignment analyzed by human experts from the list below:

{{ new_environment_logics }}

You should respond in format as follows:

```
<review> Your review of each expert output one by one </review>
<expert_id> id of the selected expert output, only the number </expert_id>
```

Optimizer Prompt Template of Interface Generation

User message:
In modern benchmarks evaluating LLM Agent reasoning capabilities, human designers create an Environment with a set of rules defining how tasks are accomplished. These rules, referred to as the Environment's World Model, specify the sequence of actions required to achieve specific outcomes. For example, the Environment's World Model might dictate that certain actions (e.g., operating on a receptacle) can only be performed after prerequisite actions (e.g., moving to the receptacle).

Meanwhile, the Agent operates based on its own World Model, which it constructs by interpreting the task and environment prompts. The Agent first determines its high-level reasoning intent—its understanding of what needs to be done—and then selects actions according to its internal World Model. However, because the Environment's World Model is manually crafted and may not be fully conveyed through prompts, the Agent's World Model might differ, leading to unexpected behavior. For instance, the Agent might choose an action that aligns with its intent but violates the Environment's rules, or it might misinterpret feedback due to insufficient information from the Environment.

We define a misalignment between the Environment's World Model and the Agent's World Model as a situation where:

- The Environment provides feedback that does not sufficiently clarify its World Model, leaving the Agent unable to adjust its understanding of the rules.

Your task is to refine the environment's behavior based on the misalignment identified by the AnalysisAgent, ensuring the Agent's true intentions are executed and its reasoning capabilities are fairly assessed.

Experimental Environment Evaluation Template

```python
{{ experimental_template }}
```

In this template, the function 'InferRules' is used to define the environment rules. The function 'WrapStep' handles post-processing of the Agent's actions (e.g., splitting them into multiple steps, performing pre-checks, returning more detailed feedback, etc.). This function should not interfere with the Agent's own reasoning. There current implementation is as follows:

```python
{{ WrapStep }}
```

Environment Logics and Misalignment Analyzed by AnalysisAgent Previously

{{ last_environment_logics }}

New Environment Logics and Misalignment Analyzed by AnalysisAgent

{{ new_environment_logics }}

Your Task

Based on the misalignments identified by the AnalysisAgent, you need to refine and enhance the 'InferRules' function and 'WrapStep' function to align the Environment's World Model with the Agent's actions and provide clearer feedback. Your output should present the new versions of these functions, ensuring the Agent's high-level reasoning intent is preserved.
Please ensure you follow these requirements:

1. **Function Signature**
The function signature must be:
```python
def InferRules(init_obs, task)
```
- init_obs: str, the initial observation from the environment, containing all receptacles.
- task: str, the task description.

```
def WrapStep(env, init_obs, task, agent_action: str, logger)
```

2. **Return Values**
The 'InferRules' function's return value must be a string that describes the environment rules.

The 'WrapStep' function's return value must be three items:
```python
obs: str, reward: bool, done: bool
```

3. **'env.step' Usage**
The only permitted usage pattern for 'env.step' is:
```python
obs, reward, done, info = env.step([agent_action])
obs, reward, done = obs[0], info['won'][0], done[0]
```
No alternative usage forms are allowed. Each call to env.step causes an irreversible

change to the environment state; actions must therefore be chosen carefully.

4. **Package Imports**
You may import other packages if necessary, but you must include all imports in your code.

5. **Multiple Calls and Conditional Returns**
You are free to call ‘env.step‘ multiple times or return different ‘obs‘ depending on ‘agent_action‘ or the outcomes of these calls.

6. **You can use logger.debug**
You can use ‘logger.debug‘ to log any information you find useful. The logging will be captured and returned to you in the future for further analysis.

7. Do not modify any aspects not explicitly identified by the AnalysisAgent in the “New Environment Logics and Misalignment Analyzed by AnalysisAgent” section.

8. You must use the following approach when addressing the identified misalignment:
- For each action defined in environment, provide clear, informative, and sufficient feedback from the environment whenever an invalid action is attempted, guiding the Agent toward understanding and adhering to the environment’s rules.

9. **Output Format**
You must provide the output strictly in the following format:
<thought>YOUR_THOUGHT_PROCESS_HERE<
<code>YOUR_CODE_HERE</code>

Please ensure your final answer follows these guidelines so that we can accurately bridge the misalignment and allow the environment to execute the Agent’s true intentions.

Optimizer Prompt Template of Experimental Verification

User message:
Now you should conduct simulation experiments in the simulator to verify if the ‘InferRules‘ and ‘WrapStep‘ function you provided is correct for the new environment logics and misalignment analyzed by the AnalysisAgent.

You must perform sufficient experiments to confirm or refute your suspicion. Here are the operations you can use:

1. init_simulator(task_id: str)
- Initializes a new simulator for the specified ‘task_id‘.
- ‘task_id‘ must be in the format ’int-int’ where the first int $\in [0, 5]$.
- The different task types are mapped as follows:

0: ’pick_and_place’,
1: ’pick_clean_and_place’,
2: ’pick_heat_and_place’,
3: ’pick_cool_and_place’,
4: ’look_at_or_examine_in_light’,
5: ’pick_two_obj_and_place’

- All subsequent operations occur within this initialized simulator.

2. reset_simulator()
- Resets the current simulator to its initial state.

3. execute_agent_action(agent_action: str)
- Executes an agent action using the ‘WrapStep‘ function you generated.

4. change_last_action_observation(obs: str)
- Updates the last observation returned by the simulator to the specified ‘obs‘.
- This is useful for simulating the agent’s next action in a different environment feedback context.

5. get_next_agent_action()
- Retrieves the next action that the real Agent would perform under the current

simulation conditions.
- Note: The Agent's choice of the next action is based on the current environment state, including the outcomes of any previous 'step()' or 'get_next_agent_action()' call, along with the latest observations.

6. run_task(task_id: str)
- Runs the entire task in the simulator and returns the running log.
- After running the whole task, you need to call 'init_simulator' or 'reset_simulator' to reinitialize the simulator for further operations.

If you believe you have reached a conclusion from your experiments, provide it in this format:

<thought> Your reasoning here </thought>
<if_need_refine> True/False </if_need_refine>
<refine_strategy> Your strategy for refining the WrapStep function, if if_need_refine is True </refine_strategy>

If you need to carry out more operations in the simulator, respond in the following format, specifying exactly one operation per turn:

<thought> Your reasoning here, you should consider all hypotheses if the simulation result is not as expected </thought>
<action> The single operation you wish to perform (e.g., init_simulator(task_id="xy"), step(action="x"), execute_agent_action(agent_action="x"), etc.) </action>

Optimizer Prompt Template of Reranking Interface Generation (Ablation Stuty)

User message:
In modern benchmarks evaluating LLM Agent reasoning capabilities, human designers create an Environment with a set of rules defining how tasks are accomplished. These rules, referred to as the Environment's World Model, specify the sequence of actions required to achieve specific outcomes. For example, the Environment's World Model might dictate that certain actions (e.g., operating on a receptacle) can only be performed after prerequisite actions (e.g., moving to the receptacle).

Meanwhile, the Agent operates based on its own World Model, which it constructs by interpreting the task and environment prompts. The Agent first determines its high-level reasoning intent—its understanding of what needs to be done—and then selects actions according to its internal World Model. However, because the Environment's World Model is manually crafted and may not be fully conveyed through prompts, the Agent's World Model might differ, leading to unexpected behavior. For instance, the Agent might choose an action that aligns with its intent but violates the Environment's rules, or it might misinterpret feedback due to insufficient information from the Environment.

We define a misalignment between the Environment's World Model and the Agent's World Model as a situation where:
- The Environment provides feedback that does not sufficiently clarify its World Model, leaving the Agent unable to adjust its understanding of the rules.

Now other human experts have generated a set of code patches to address the misalignment between the Environment's World Model and the Agent's World Model. Your task is to evaluate these patches and select the best one.

Experimental Environment Evaluation Template

```python
{{ experimental_template }}
```

```

In this template, the function 'InferRules' is used to define the environment rules. The function 'WrapStep' handles post-processing of the Agent's actions (e.g., splitting them into multiple steps, performing pre-checks, returning more detailed feedback, etc.). This function should not interfere with the Agent's own reasoning. There current implementation is as follows:

```python
{{ WrapStep }}
```

Environment Logics and Misalignment Analyzed by AnalysisAgent Previously

{{ last_environment_logics }}

New Environment Logics and Misalignment Analyzed by AnalysisAgent

{{ new_environment_logics }}

Your Task

Choose the best code from the following options to address the misalignment between the Environment's World Model and the Agent's World Model:

{{ code_patches }}

You should respond in format as follows:
```
<review> Your review of each code one by one </review>
<code_id> id of the selected result, only the number </code_id>
```
```

We present the prompt template of the Vanilla agent in ALFWorld to illustrate the usage of the InferRules. For the prompt templates of other agent methods and benchmarks, please refer to the supplemental materials.

Vanilla Agent Prompt Template in ALFWorld

System message:
You are an AI assistant solving tasks in a household environment. Your goal is to break down complex tasks into simple steps and plan your actions accordingly.

Action Space

In this environment, you have a set of high-level actions at your disposal, each corresponding to a typical household activity. These actions are:

- look: look around your current location
- inventory: check your current inventory
- go to (receptacle): move to a receptacle
- open (receptacle): open a receptacle
- close (receptacle): close a receptacle
- take (object) from (receptacle): take an object from a receptacle
- move (object) to (receptacle): place an object in or on a receptacle
- examine (something): examine a receptacle or an object
- use (object): use an object
- heat (object) with (receptacle): heat an object using a receptacle
- clean (object) with (receptacle): clean an object using a receptacle
- cool (object) with (receptacle): cool an object using a receptacle
- slice (object) with (object): slice an object using a sharp object

Although each action may internally consist of multiple embodied steps (e.g., walking to the sink, turning a knob, etc.), from your perspective you need only provide one high-level action at a time.

Instructions

Single Action per Turn
At each step, you must respond with exactly one action (i.e., the next "thought"). Use the format:
ACTION [object/receptacle specifier]
ACTION [object/receptacle specifier]
For example:
take apple from table
or
go to kitchen.

Environment Feedback
After you provide your single action, the environment will automatically execute it and return the resulting observation. You then decide on your next action based on the updated state.

Reasoning (Chain of Thought)
You may use hidden reasoning to figure out the best next step. However, only output the single action that represents your decision. Do not reveal your entire chain of thought.

Continue Until Task Completion
You will iterate this process—receiving the environment's feedback, deciding on the next action, and outputting a single action—until the task is finished.

Environment Rule

{InferRules(init_obs, task)}

User message:
Task

{initial_obs}

Begin by examining the environment or taking any initial steps you find relevant. Remember, provide only one action each time.