Close the Loop: Synthesizing Infinite Tool-Use Data via Multi-Agent Role-Playing

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Abstract

Enabling Large Language Models (LLMs) to reliably invoke external tools remains a critical bottleneck for autonomous agents. Existing approaches suffer from three fundamental challenges: *expensive human annotation for high-quality trajectories, poor generalization to unseen tools, and quality ceilings inherent in single-model synthesis that perpetuate biases and coverage gaps*. We introduce **InfTool**, a fully autonomous framework that breaks these barriers through self-evolving multi-agent synthesis. Given only raw API specifications, InfTool orchestrates three collaborative agents (User Simulator, Tool-Calling Assistant, and MCP Server) to generate diverse, verified trajectories spanning single-turn calls to complex multi-step workflows. The framework establishes a closed loop: synthesized data trains the model via Group Relative Policy Optimization (GRPO) with gated rewards, the improved model generates higher-quality data targeting capability gaps, and this cycle iterates without human intervention. Experiments on the Berkeley Function-Calling Leaderboard (BFCL) demonstrate that InfTool transforms a base 32B model from 19.8% to **70.9% accuracy (+258%)**, surpassing models 10× larger and rivaling Claude-Opus, and entirely from synthetic data without human annotation.

1 Introduction

Tool calling (Schick et al., 2023) in Figure 1 is pivotal for transforming LLMs into autonomous agents to interactive with external system and accomplish tasks beyond the intrinsic knowledge. However, reliable and generalizable tool callings remain 3 fundamental challenges: **1) Data Scarcity**, where high-quality interaction trajectories require expensive human annotation and post verification; **2) Limit Generalization**: Static datasets fail to
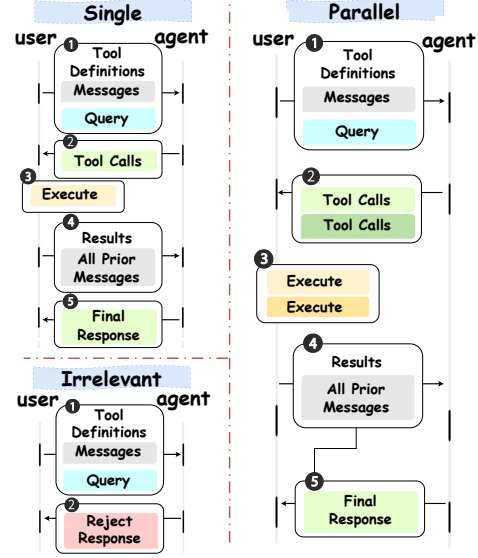

Figure 1: MCP-based tool calling across three scenarios.

adapt unseen tools during training; **3) Quality Cell**: synthesizing training data with LLMs traps performance in a local optimum, inheriting synthesis model biases and blind coverage.

To address these challenges, we propose **InfTool**, a fully **Human-Annotation-Free** self-evolving framework that establishes a closed-loop system of synthetic data generation and iterative model optimization. Specifically, InfTool tackles **Data Scarcity** by employing a role-playing multi-agent system (User Simulator, Tool Agent, and Server Simulator) to automatically generate high-quality interaction trajectories from raw API specifications, eliminating expensive human annotation. To overcome **Limited Generalization**, our framework synthesizes training data directly from MCP tool schemas, enabling adaptation to unseen tools without requiring static datasets. To break through the **Quality Ceiling**, we integrate GRPO (Shao et al., 2024) with a gated composite reward mechanism that ensures synthesized data quality continuously improves: the optimized model generates increasingly sophisticated trajectories, which in turn drives further policy refinement, creating a

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[*] Equal contribution.
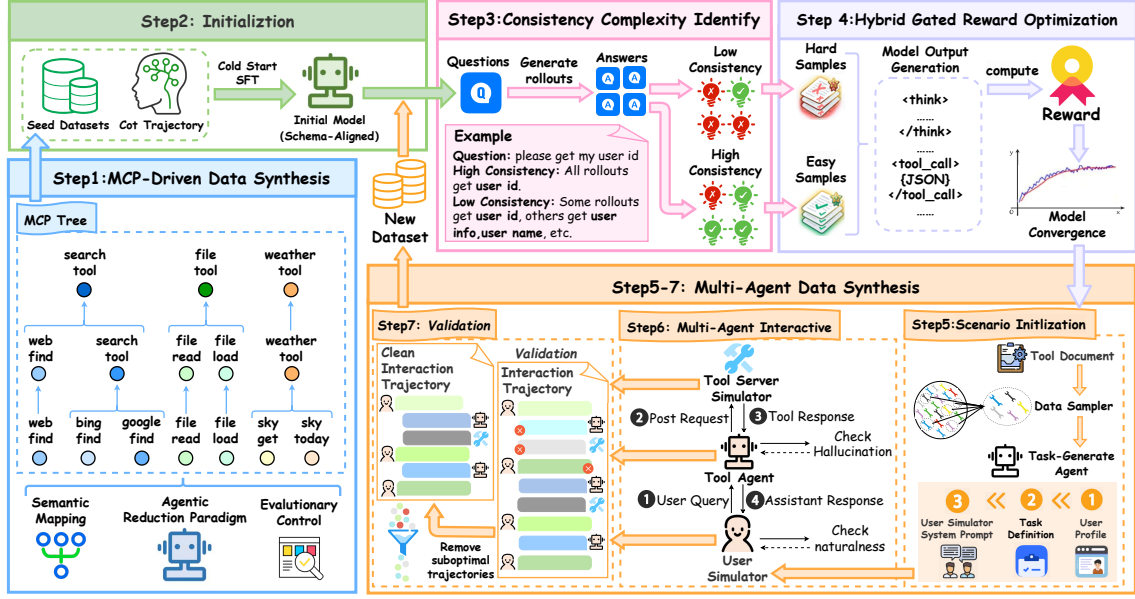[†] Corresponding author.

Figure 2: Overview of our framework. Step 1: Build MCP tool definitions from raw APIs. Step 2: Cold start Supervised Fine Tuning (SFT) (Radford et al., 2018). Step 3: Rollout evaluation to categorize samples. Step 4: GRPO training. Step 5-6: Multi-agent role-play (User, Agent, Server) generates complex trajectories. Step 7: Self-reflection filtering.

self-reinforcing virtuous cycle that transcends the limitations of single-model synthesis.

Our main contributions are as follows: **(1) Framework Innovation:** We introduce InfTool, a self-evolving framework that utilizes simulated multi-agent role-playing to generate high-quality tool-calling data purely from API specifications, eliminating the need for human annotation and post-hoc verification. **(2) Scalable Synthesis**: We propose a methodology for synthesizing training data at unbounded scale with controllable complexity through iterative GRPO-driven optimization, effectively resolving data scarcity and quality ceiling issues in multi-turn scenarios. **(3) State-of-the-Art Performance:** Experiments demonstrate that InfTool improves the base model (Qwen2.5-32B) performance from 19.8 to 70.9 on BFCL (+**258.08%**). Notably, InfTool-32B outperforms strong open-source baselines (DeepSeek-AI, 2025; Qwen Team, 2025) and achieves competitive performance with leading proprietary models (Anthropic, 2024; OpenAI et al., 2023).

2 Methodology

We first introduce the preliminary concepts of tool use and the RL (Watkins, 1989) which underpin our system. Subsequently, we present the ROLE-PLAYING MULTI-AGENT FRAMEWORK (Li et al., 2023), an integrated system designed for high-fidelity data synthesis. Finally, we elaborate on the iterative self-evolving mechanism that acts as

the framework's engine, driving continuous capability enhancement.

2.1 Preliminaries

Tool Use and MCP Agentic tool use capability is formally defined as the policy π mapping a user query q and a context C to a structured action space $\mathcal{A}$. In our work, we adopt the MCP, a standardized interface that decouples the AI model as the client from the data sources as the server. Within MCP, a tool call is represented as a tuple $t = (f, \mathbf{a})$, where f is the function identifier and $\mathbf{a}$ represents the arguments conforming to a strict JSON schema $\mathcal{S}_f$. The fundamental challenge in MCP training is ensuring the model's generated $\hat{\mathbf{a}}$ strictly adheres to $\mathcal{S}_f$ while satisfying the semantic intent of q.

Group Relative Policy Optimization (GRPO) To optimize the model's reasoning and tool-invocation precision, we employ GRPO (Shao et al., 2024), a policy optimization algorithm that eliminates the need for a separate value network, thereby reducing memory overhead. GRPO optimizes the policy π_θ by maximizing the objective:

$$\mathcal{J}(\theta) = \mathbb{E}\left[\frac{1}{G}\sum_{i=1}^{G}\min\left(\rho_i A_i, \right.\right.$$
$$\left.\left. \text{clip}(\rho_i, 1-\epsilon, 1+\epsilon)A_i\right) - \beta\mathbb{D}_{\text{KL}}(\pi_\theta||\pi_{\text{ref}})\right]$$

$$(1)$$

where $\mathbb{E}$ denotes $\mathbb{E}_{q \sim P(Q), \{o_i\} \sim \pi_{\theta_{\text{old}}}}$, and $\rho_i = \frac{\pi_\theta(o_i|q)}{\pi_{\theta_{\text{old}}}(o_i|q)}$ is the importance ratio. Here, $\pi_{\theta_{\text{old}}}$ is the sampling policy, G is the group size, and A_i is the advantage. This compact formulation supports efficient iterative updates on self-generated data.

2.2 Role-Playing Multi-Agent Data Synthesis

Framework Overview We propose a self-evolving role-playing multi-agent framework that unifies high-quality data synthesis with iterative model refinement. In Figure 2, the framework operates as a closed loop: 1) **MCP Driven Data Synthesis** employs a multi-agent system to construct complex interaction trajectories from raw API definitions. 2) **Iterative Self-Evolving Training Loop** utilizes the synthesized data and GRPO to update the model, and the model in turn empowers the agents to generate even higher-quality data in subsequent iterations.

MCP Tree We initialize the pipeline by ingesting 17,713 candidates from RapidAPI[1]. We propose an iterative refinement framework for a rigorous foundation, designed to disambiguate unclear MCP Tool definitions and merge functionally redundant entries. Formally, let $\mathcal{T}^{(r)}$ denote the toolset at the r-th iteration. For each tool $t_i \in \mathcal{T}^{(r)}$, we compute its semantic embedding $\mathbf{e}_i$. Tools exhibiting high semantic overlap are aggregated into K candidate clusters $\mathcal{C} = \{\mathcal{C}_1, \ldots, \mathcal{C}_K\}$. A cluster $\mathcal{C}_k$ is defined as a subset where elements maintain a pairwise cosine similarity exceeding a threshold δ:

$$\mathcal{C}_k = \{t_i \in \mathcal{T}^{(r)} \mid \exists t_j \in \mathcal{C}_k, j \neq i, \cos(\mathbf{e}_i, \mathbf{e}_j) > \delta\} \quad (2)$$

Subsequently, an LLM acts as a semantic discriminator to partition $\mathcal{C}_k$ into a redundant subset $\mathcal{R}_k$ and a unique subset $\mathcal{U}_k$. The refined toolset $\mathcal{T}^{(r+1)}$ is derived by synthesizing a consolidated definition $\hat{t}$ for the redundant subset via a generative abstraction operator $\mathcal{A}_{\text{gen}}$:

$$\mathcal{T}^{(r+1)} = \bigcup_{k=1}^{K} \left(\mathcal{U}_k \cup \{\mathcal{A}_{\text{gen}}(\mathcal{R}_k)\} \right) \quad (3)$$

This procedure yields 3,059 high-fidelity synthetic MCP Tools.

Hierarchical Data Synthesis We synthesize the data in two stage. **Single-Turn Synthesis** Single-turn synthesis addresses three specific sub-tasks:

standard execution, parallel tool execution, and irrelevance detection. We implement a streamlined pipeline where selected tool schemas serve as context for generating user queries. An agent executes the task, producing a trajectory subjected to rigorous verification. **Multi-Turn Synthesis via Role-Playing** For complex scenarios, we developed an interactive multi-agent playground populated by three roles: an User Simulator, a Tool Agent (MCP Client), and a MCP Server Simulator. A Task Generation Agent creates dynamic scenarios defined by five dimensions: user profile, known/unknown information, user need, and difficulty. The agents interact to resolve unknown information progressively, generating 3 to 5 round interaction trajectories that enforce strict logical dependencies.

Quality Assurance Mechanism We implement a dual-layer quality assurance mechanism to guarantee fidelity: **1) Intrinsic Self-Reflection (In-Trajectoral):** Operating in real-time, this stage enforces stylistic constraints Ψ_{style} for the user agent and strict MCP schema compliance for the client agent. The corrected response o_t' is generated via a self-correction function

$$o_t' = \mathcal{S}(o_t \mid \Psi_{\text{style}}(o_t), \Psi_{\text{schema}}(o_t)) \quad (4)$$

This effectively rectifies errors such as hallucinated tool requests or argument violations. **2) Multi-Agent Validation (Post-Trajectoral):** Upon trajectory completion, validator agents $V = \{v_1, \ldots, v_M\}$ leverage a voting-deliberation-correction loop. The final accepted trajectory $\mathcal{L}^*$ is derived by minimizing redundancy $R(\cdot)$ through consensus:

$$\mathcal{L}^* = \mathcal{M}_{\text{consensus}}(\mathcal{L} \mid \{v_i\}_{i=1}^{M}) \quad (5)$$

2.3 Self-Evolution Training Loop

To enable the framework to progressively enhance its own capabilities, we integrate a self-evolving training loop. This component is not merely a downstream application but the engine that powers the "Self-Evolving" nature of our role-playing framework.

Complexity Stratification At each iteration t, the agent's policy π_{θ_t} is evaluated to stratify the dataset $\mathcal{D}_t$ into "Easy" and "Hard" subsets based on an execution consistency score c_i:

$$\mathcal{D}_t^{\text{Hard}} = \{(\mathbf{q}_i, \mathbf{a}_i^*) \mid c_i < \gamma\} \quad (6)$$
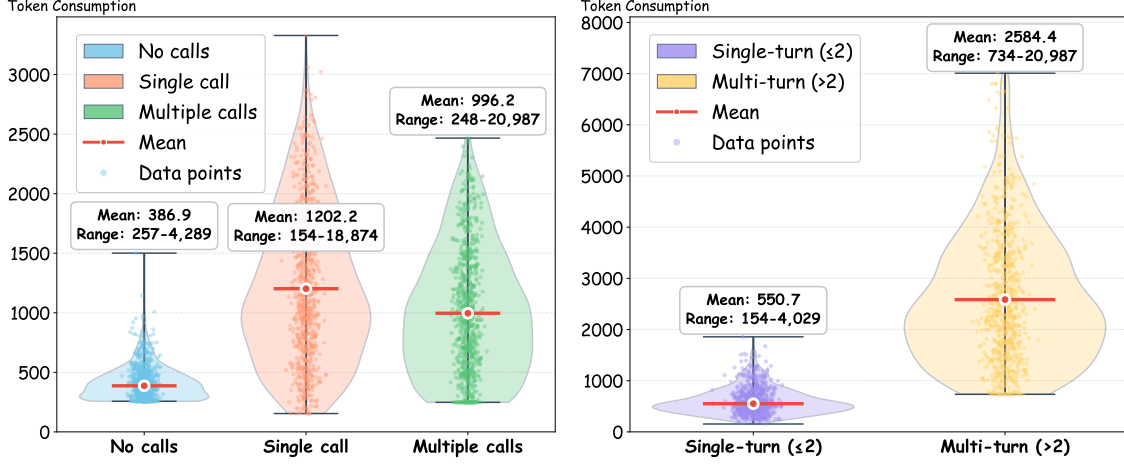
Figure 3: Token consumption distribution across tool-call categories and conversation lengths. The left panel shows token requirements for different tool-call frequencies (no calls, single call, multiple calls), while the right panel contrasts single-turn versus multi-turn conversations. Box plots indicate quartiles, with whiskers extending to the 5th and 95th percentiles.

The "Hard" subset defines the learning frontier for the next cycle.

Gated Composite Reward Policy Optimization
We update the policy using GRPO with a specialized composite reward function $R(\mathbf{T})$ that aligns the model with the MCP protocol:

$$
\begin{aligned}
R(\mathbf{T}) = {} & R_{\text{format}}(\mathbf{T}) + R_{\text{tool}}(\mathbf{a}, \mathbf{a}^*) \\
& + \mathbb{I}\big(R_{\text{tool}} > \tau_t\big) \cdot \alpha \cdot R_{\text{teacher}}(\mathbf{r}; \mathbf{q})
\end{aligned}
\tag{7}
$$

here, R_{format} rewards syntactic validity (e.g., correct `<think>` and `<tool_call>` tags), while R_{tool} measures execution fidelity. Crucially, a reasoning quality reward R_{teacher} is *gated* ($\mathbb{I}$), meaning it is only awarded when correct execution, strictly binding reasoning improvements to functional utility.

Adaptive Data Injection The cycle closes by engaging the *Multi-Agent Data Synthesis Module* (described in Sec. 2.2) to generate new training samples $\mathcal{D}_t^{\text{new}}$ specifically targeting the identified competency frontiers in $\mathcal{D}_t^{\text{Hard}}$. This creates a self-sustaining loop where improved agents generate superior data, which in turn trains stronger agents.

3 Data Analysis

Computational Complexity Analysis Analysis identifies three interaction patterns with distinct computational demands. No tool-calls are simplest, while single tool-calls, comprising 53.7% of the dataset, are more demanding. Multi tool-calls show similar average complexity but greater consistency. Conversation length further amplifies load: multi-turn dialogues require approximately four times the tokens of single-turn ones in Figure 3.
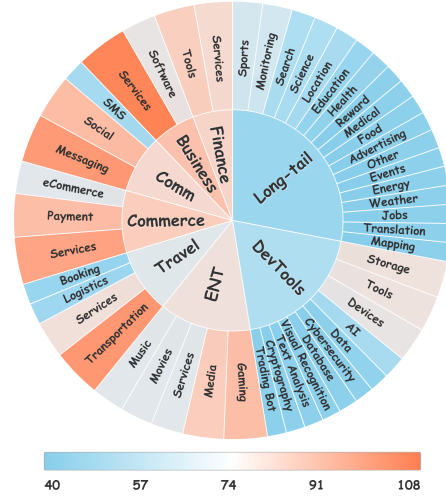

Figure 4: Domain distribution in the training dataset.

Dynamic Dataset Composition and Evolution
Our training corpus evolves dynamically through the self-evolving RL loop. The initial seed dataset spans 15 primary domains and a long-tail of 35 additional categories, with broad coverage across diverse application scenarios. Critical baseline analysis reveals that 82.83% of MCP tools require parameter specifications, establishing a significant benchmark of complexity for semantic parsing. Domain-specific analysis indicates particularly high parameter requirements in structured fields such as Finance, Travel, and Sports in Figure 4.

Multi-Turn Conversation Statistics We further analyze multi-turn dialogues (with more than one turn) in our dataset, totaling 4,965 conversations. The number of turns ranges from 2 to 15, with an average of 7.78 turns and a median of 8 turns.
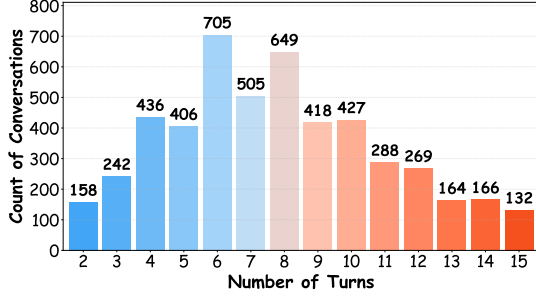
Figure 5: Distribution of Conversation Turns.

Most conversations are concentrated in the 6–8 turn range, which accounts for 37.44% of the dataset. Overall, 62.46% of multi-turn dialogues have 8 turns or fewer, while longer conversations exceeding 10 turns represent 20.52%, highlighting the presence of substantial long-horizon interactions that challenge contextual maintenance and sequential tool usage in Figure 5.

4 Experiment

4.1 Experiment Setup

Hardware Infrastructure We conduct our experiments on a robust computational infrastructure running Ubuntu 22.04, equipped with an Intel Xeon (R) Gold 6348 CPU @2.60GHz, 8 NVIDIA H800 GPUs, and 528 GB of memory, providing substantial computational resources for large scale model training and inference operations across multiple experimental phases.

Model Deployment Our experimental pipeline employs three models for different phases: EmbeddingGemma for semantic clustering, Qwen3-Coder-30B-Instruct for tool refinement and data generation, and DeepSeek-R1 for chain-of-thought trajectory generation during cold-start initialization. We conduct supervised fine-tuning and iterative self-evolving RL across two model scales: Qwen2.5-7B and Qwen2.5-32B.

Training Setup During SFT stage, we adopt a full parameter training strategy with 512 global batchsize, 1e-5 learning rate and train for 3 epochs under BF16 (Kalamkar et al., 2019) precision to improve both speed and numerical stability. During the RL stage, we adopt a data sampling strategy with 0.7 generation temperature and generate 1000 steps per iteration at 1024 global batchsize.

4.2 Evaluate Metric

To rigorously assess multi-agent function calling capabilities, we evaluate our models on BFCL (Yan
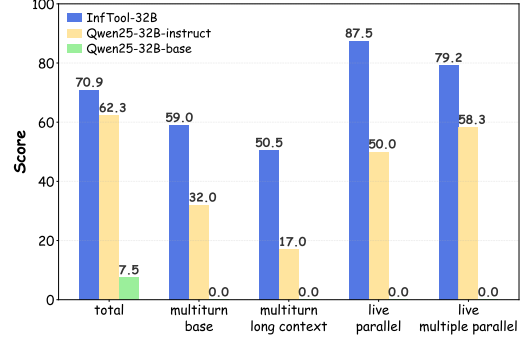

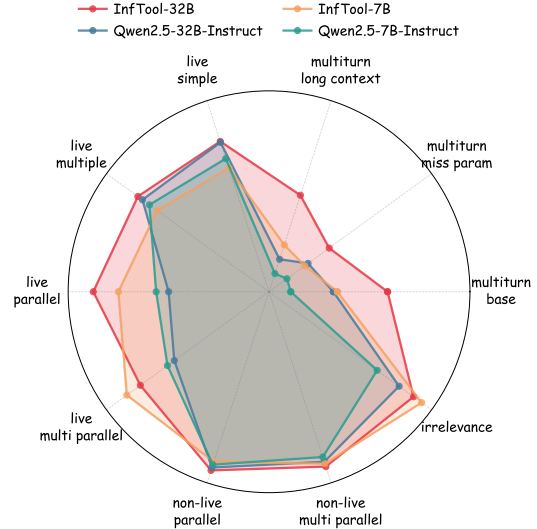Figure 6: Comparison of InfTool and baselines.

Figure 7: Analysis of InfTool and baselines.

et al., 2024). BFCL V3 is chosen for its advanced multi-turn and multi-step assessment capabilities, which test iterative problem solving in complex scenarios like state inconsistencies. **Notes:** Although BFCL released version 4 earlier, technical issues prevented us from reproducing most of the results reported for this version in our experiments. Specifically, all newly added test items yielded zero values. Therefore, we restrict our experimental evaluation to version 3.

4.3 Main Result

Trained on our proprietary dataset, our **InfTool-7B** model achieves a Total BFCL score of 61.7, surpassing **GPT-5.2** (60.4). Meanwhile, the **InfTool-32B** model achieves a score of 70.9, ranking as the top-performing open-source model in Table 1, outperforming **Kimi-K2-Instruct** (70.6) and trailing only top-tier proprietary models like **Claude-Opus**. Notably, our approach yields significant improvements over baselines. In multi-turn scenarios, InfTool-32B (59.0) surpasses the Qwen2.5-32B-Instruct baseline (32.0) by approximately 84% and outperforms the specialized coding model, Qwen3-Coder-30B-A3B-Instruct (36.0), by a substantial

Model	Size	Total	Multi-Turn				Non-Live				Live				Relevance	Irrelevance
			Base	Miss Func	Miss Param	Long Cont.	Simple	Multiple	Parallel	Multi Para.	Simple	Multiple	Parallel	Multi Para.		
Closed-source Model																
Claude-Opus-4-5-20251101	🔒	**78.9**	**81.0**	64.0	**58.0**	70.5	76.8	95.5	93.5	88.5	86.5	78.1	**87.5**	75.0	62.5	84.7
Claude-Sonnet-4-5-20250929	🔒	77.0	69.0	**65.0**	52.5	59.0	72.6	95.5	94.5	**92.0**	89.5	78.9	**87.5**	83.3	68.7	**86.6**
Gemini-3-Pro-Preview	🔒	76.8	69.0	63.0	56.5	64.0	75.5	94.0	91.0	82.5	87.6	**80.4**	75.0	79.1	75.0	77.8
GPT-5.2-2025-12-11	🔒	60.4	36.5	18.0	27.5	30.5	72.9	88.0	89.0	77.5	71.7	70.3	68.7	58.3	75.0	79.4
GPT-o3-2025-04-16	🔒	40.4	16.5	11.5	14.5	16.5	74.5	87.0	0.0	0.0	70.5	67.6	0.0	0.0	**81.2**	86.1
Grok-4-1-fast-reasoning	🔒	75.2	70.5	59.5	43.0	62.5	**77.5**	93.0	92.5	90.0	84.1	77.3	75.0	75.0	**81.2**	79.4
Open-source 14B+ Model																
Kimi-K2-Instruct	32B/1TB	**70.3**	**62.0**	41.0	**44.5**	55.0	69.4	92.0	82.0	83.0	81.7	78.0	87.5	66.6	75.0	87.3
DeepSeek-V3.2-exp	685B	41.96	41.5	39.5	33.5	35.0	37.9	74.0	15.0	12.5	66.2	51.6	25.0	25.0	37.5	**93.1**
Qwen3-Coder-480B-A35B-Instruct	35B/480B	69.9	51.5	27.5	31.0	49.5	77.9	94.0	93.0	86.0	83.7	81.0	81.3	70.8	66.7	85.5
Qwen3-235B-A22B-Instruct	22B/235B	50.5	54.0	42.5	31.5	50.5	40.5	36.5	53.0	19.5	58.5	71.6	68.7	62.5	87.5	81.7
Qwen2.5-72B-Instruct	72B	63.8	28.0	34.0	27.5	29.0	73.6	95.0	92.0	88.5	74.0	77.5	50.0	62.5	72.2	80.5
Llama-3.3-70B-Instruct	70B	62.0	28.0	19.5	14.0	24.5	76.8	95.0	90.0	92.0	81.0	75.3	87.5	75.0	100.0	53.7
CoALM-70B	70B	65.1	11.0	14.0	9.0	8.5	70.2	92.0	88.5	83.0	70.5	66.5	68.7	62.5	93.7	85.6
mistral-large-2411	70B	60.2	18.5	11.5	13.0	13.5	72.0	93.5	89.5	83.5	87.2	80.7	81.2	75.0	93.7	68.9
Qwen3-32B Chat	32B	60.0	19.5	16.5	17.0	13.5	76.7	96.0	89.5	91.5	86.1	81.0	62.5	70.8	87.5	75.7
Qwen2.5-32B-Instruct	32B	62.2	32.0	25.5	24.0	17.0	65.5	92.5	92.0	89.0	78.2	77.9	50.0	58.3	66.6	80.2
Qwen3-Coder-30B-A3B-Instruct	3B/30.5B	62.6	36.0	16.0	19.5	33.0	75.3	95.0	88.0	83.5	83.3	79.5	62.5	83.3	88.9	77.0
Gemma-3-27b	27B	57.4	16.5	4.5	8.0	14.0	77.6	92.5	89.0	89.5	84.5	72.4	93.7	45.8	81.2	73.6
Granite-20b	20B	48.8	9.0	3.0	6.5	3.0	72.9	91.5	83.5	81.5	67.8	56.7	43.7	58.3	87.5	75.1
Qwen2.5-14B-Instruct	14B	59.9	29.5	25.5	21.5	19.5	65.0	96.0	79.5	86.5	75.2	74.2	68.8	62.5	72.2	76.4
Qwen3-14B Chat	14B	58.5	17.0	15.5	15.5	8.5	74.4	95.0	92.5	88.0	85.3	79.1	56.3	75.0	75.075	82.9
Open-source 0.5–14B Models																
Bielik-11B-v2.3-Instruct	11B	50.6	4.5	0.5	3.0	2.5	73.0	92.0	85.5	75.5	75.5	66.1	62.5	58.3	93.7	36.0
Falcon3-10B-Instruct	10B	55.6	6.5	9.5	5.0	5.0	70.5	93.5	88.5	87.5	77.1	76.1	50.0	41.6	93.7	32.0
Qwen3-8B Chat	8B	59.5	14.5	15.5	13.5	12.0	71.7	97.0	90.0	91.0	84.9	79.2	68.8	66.7	81.3	78.1
Granite-3.1-8B-Instruct	8B	48.7	11.5	2.0	7.5	9.0	67.3	92.0	84.0	70.0	58.5	61.8	18.7	41.6	68.7	79.9
CoALM-8B	8B	53.2	10.0	7.0	8.0	7.0	69.5	93.5	88.0	88.5	70.5	66.1	62.5	54.1	87.5	86.9
Hammer2.1-7b	7B	**59.6**	24.0	28.5	21.5	21.5	72.5	92.5	91.0	86.0	66.6	69.9	75.0	75.0	50.0	**90.1**
Qwen3-4B Chat	4B	50.9	9.5	9.0	7.0	9.5	75.2	93.0	92.5	90.0	78.3	76.3	56.3	66.7	87.5	84.9
MiniCPM3-4B-FC	4B	51.2	6.5	2.0	4.5	2.5	70.5	92.0	84.0	80.5	73.2	63.5	50.0	62.5	68.7	72.8
Qwen2.5-3B-Instruct	3B	49.7	9.0	0.0	8.0	3.5	71.4	91.0	72.5	73.0	71.3	70.0	62.5	54.2	77.8	67.3
Llama-3.2-3B-Instruct	3B	48.3	4.5	3.5	4.0	3.5	70.7	92.0	88.5	77.0	64.7	57.7	18.8	37.5	**93.8**	52.1
Falcon3-3B-Instruct	3B	36.7	1.5	0.5	0.5	1.5	56.5	69.5	67.0	25.5	57.3	54.7	25.0	33.3	81.2	32.9
Qwen2.5-1.5B-Instruct	1.5B	45.7	3.5	1.0	2.5	2.0	59.5	84.0	67.0	64.5	69.4	59.5	50.0	62.5	83.3	72.4
Arch-Agent-1.5B	1.5B	59.0	35.5	27.5	21.5	22.0	72.1	92.0	85.5	81.0	70.5	67.8	31.2	58.3	75.0	74.8
Llama-3.2-1B-Instruct	1B	16.7	0.0	0.0	0.0	0.0	44.1	50.0	43.5	14.0	30.2	6.8	0.0	0.0	43.8	53.0
Qwen3-0.6B Chat	0.6B	40.5	2.5	1.5	0.0	1.0	64.3	82.0	69.0	59.0	58.1	50.7	56.3	41.7	68.8	81.8
Qwen2.5-0.5B-Instruct	0.5B	35.7	1.0	0.0	0.5	1.0	48.4	74.5	48.5	43.0	50.0	36.6	56.3	25.0	72.2	64.6
Baselines & Our Models																
InfTool-32B	32B	70.9	59.0	29.5	37.0	50.5	70.3	95.0	93.5	91.5	78.7	81.7	87.5	79.2	66.6	88.9
InfTool-7B	7B	61.7	34.0	10.5	22.0	24.5	59.5	89.5	89.0	90.0	64.7	68.9	75.0	87.5	44.4	93.9

Table 1: Performance comparison on the Berkeley Function Calling Leaderboard (BFCL). "Total" denotes the overall accuracy.Following the leaderboard structure,metrics are categorized into Multi-Turn (including Base and error analysis).Non-Live (AST evluation),Live (Real Record), and Hallucination Measurement.Scores shown in boldface indicate the highest score for each metric.The 🔒 icon indicates that the model's parameter size is not publicly released (size locked)."-" indicates that the model was not explicitly trained for tool-calling capabilities and "!" indicates that the score is actually wrong (higher than real score).

margin. In Figure 6 and Figure 7, we compare our **InfTool-32B** against the **Qwen2.5-32B-Instruct** baseline across five dimensions. Our model consistently dominates, particularly in multi-turn reasoning (scoring **59.0** vs. 32.0) and live parallel tool execution (**87.5** vs. 50.0). The baseline's lower scores in these complex settings highlight its limitations in handling multi-turn or parallel scenarios, validating the robustness of our framework.

5 Analysis

Error Distribution Analysis Figure 8 shows where errors occur in our model. We observe an interesting pattern: The model improves well on complex tasks. For example, it achieves a **93.3%** improvement rate on Complex Length scenarios. However, regarding the substantial volume of "Sim-

ple" tasks in the benchmark, a significant number of errors persist despite the notable improvements. This happens because of **data volume**: the test set contains far more simple tasks (like Simple Parameter Types) than complex ones. Even though simple tasks have lower error rates, their large quantity means they still contribute the most total errors.

Data Scaling In Figure 9, we investigated the scaling effect by employing varying amounts of synthetic data by SFT, ranging from 1,000 to 50,000 samples. We observed significant improvements; notably, at 50k samples, the model achieves performance comparable to the our RL model. However, given that the RL method utilizes 5k samples per iteration, the SFT approach required approximately twice the total data volume to attain equivalent performance.
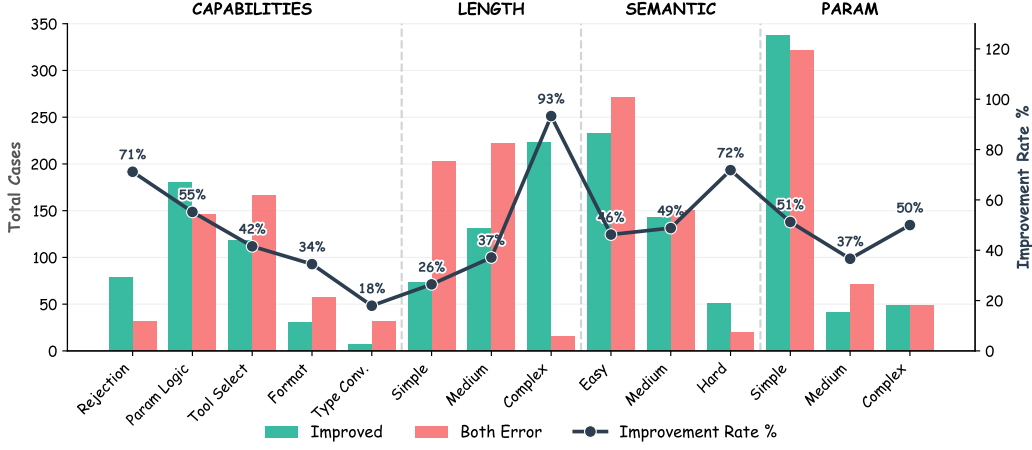
Figure 8: **Unified Performance Landscape: Volume vs. Efficiency.** This dual-axis chart integrates capability metrics with complexity dimensions. The **Bars** represent the absolute volume of cases, divided into Improved samples (green) and Persistent Errors (red, indicating failures in both Instruct and `InfTool` models). The **Line** tracks the Improvement Rate (Efficiency), revealing the model's improvement across different domains.
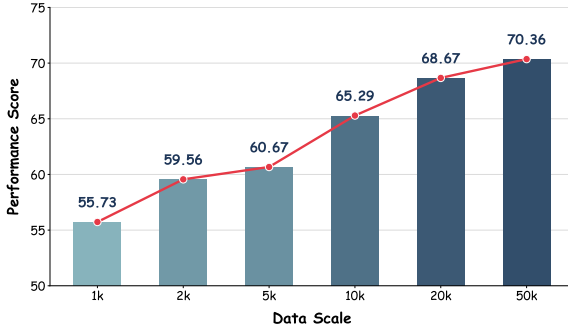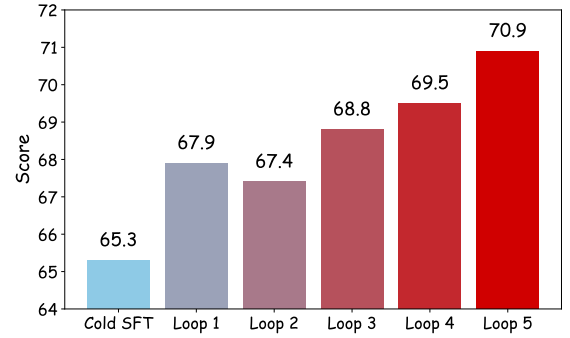

Figure 9: Influence of data scale.

Figure 10: Performance evolution on BFCL across the iterative self-evolving training stages.

Domain	Baselines	InfTool	Improvement
Retail	40.0	67.0	+67.5%
Airline	26.0	60.0	+130.8%
Telecom	21.0	67.5	+221.4%

Table 2: Performance on τ^2-Bench (Success Rate %).

Out of Distribution Evaluation To evaluate the model's capability in complex environments, we benchmarked our approach against the official τ^2-Bench (Yao et al., 2025). This benchmark is particularly challenging as it requires the agent to guide a user simulator through state-dependent tasks. As illustrated in Table 2, our training framework yields substantial gains over the Instruct baseline. These results demonstrate that our specialized training strategy enables a smaller model to rival or exceed the performance of significantly larger general-purpose models in collaborative troubleshooting scenarios.

Ablation Study on RL Figure 10 illustrates the performance trajectory from an SFT baseline of 65.3 to a final score of 70.9. The policy adapts in subsequent rounds, showing a robust upward trend.

Category	w/o MCP Tree	InfTool (Full)	Δ
Overall	55.21	**70.90**	**-15.69**
Live			
Live Parallel AST	50.00	87.50	-37.5
Multi-Turn Interactions			
Multi Turn Base	20.00	59.00	-39.00
Multi Turn Miss Func	13.00	29.50	-16.50
Multi Turn Miss Param	13.50	37.00	-23.50
Multi Turn Long Context	11.00	50.50	-39.50
Detection Accuracy			
Irrelevance Detection	61.02	88.90	-27.88

Table 3: MCP Tree ablation in multiple categories.

This cumulative +5.6 improvement validates our core hypothesis: a closed-loop system where improved agents synthesize superior data effectively drives continuous capability enhancement.

The Impact of MCP Tree To investigate the contribution of the MCP Tree our hierarchical tool refinement and deduplication module we conducted an ablation study. We compared our full model against a variant trained on raw, unrefined API data

Data Type	Total Hallucinations	Resolved	Failed
Single Turn	5,351	4,690	661
Multi Turn	3,399	410	2,989

Table 4: Data Generation Hallucination Statistics.

Metric	Origin Data	No Self-Refine Data	Change (%)
Miss Func	29.5	9.0	-69.4
Miss Param	37.0	6.0	-83.8
Nonlive Multi Para.	91.5	34.5	-62.2
Live Parallel	87.5	37.5	-57.1
Irrelevance	88.9	4.86	-94.5

Table 5: Performance Metrics Comparison Before and After Removing Self-Refine.

without semantic merging or disambiguation. In Table 3, the absence of the MCP Tree leads to a significant performance degradation, with the overall score dropping from 70.9 to 55.2.

Hallucination Analysis and Ablation Study In Table 4 and 5, to assess the impact of data quality, we analyzed hallucination patterns and conducted an ablation study on the Self-Reflection mechanism. The synthesis of multi-turn dialogues proved highly error-prone, with a low correction success rate (12.06%) compared to single-turn data (87.65%), necessitating the discard of many samples. The ablation study confirms the mechanism's critical role: its removal caused consistent performance degradation, most sharply in the irrelevance metric (dropping from 88.9 to 4.86). This indicates that without self-reflection, the model learns to invoke tools indiscriminately, severely harming generalization.

Rejection Analysis We implemented a multi-agent voting mechanism to detect user rejections of incorrect tool use, even without overt hallucinations. This triggered trajectory pruning in 82 multi-turn instances (1.2% of cases). While proportionally small, these unproductive attempts impacted token consumption and context efficiency.

6 Related Work

LLM and Agents LLMs (Yang et al., 2025c,a) have evolved from static knowledge repositories into dynamic agents capable of autonomous reasoning and interaction (Liu et al., 2024; Zhang et al., 2025b, 2024; Wang et al., 2023a; Zhang et al., 2025a). Frameworks like ReAct (Yao et al., 2023) and AutoGPT (Richards, 2023) enable this

by interleaving reasoning traces with executable actions to navigate dynamic workflows. However, despite these advancements, agentic scalability remains constrained by rigid prompt engineering and reliance on model-specific implementations.

Interface Standardization, Function Calling, and Evaluation To bridge the gap between agents and applications, the field is shifting from ad-hoc API wrappers to unified protocols. The recent MCP addresses integration complexity by decoupling clients from servers via a standardized schema (Lu et al., 2025). Within this ecosystem, instruction-tuning for *Function Calling* enables modular workflows, though generating accurate solution paths remains challenging; ambiguous API descriptions often lead to execution failures (Wang et al., 2023b; Wu et al., 2025). While pipelines like APIGen (Chen et al., 2024b) improve single-turn data quality, evaluation methodologies have had to evolve alongside these capabilities. Modern benchmarks have moved beyond simple API coverage: the **Berkeley Function Calling Leaderboard** (Yan et al., 2024) provides rigorous metrics for complex scenarios, while τ**-bench** (Yao et al., 2024) specifically evaluates the temporal reasoning required for sequential tool usage (Yang et al., 2025b).

Synthetic Data Synthetic data generation serves as a scalable alternative to manual collection for fine-tuning LLMs (Patil et al., 2023; Qin et al., 2023). Multi-agent frameworks like BUTTON (Chen et al., 2024a) and ToolACE (Huang et al., 2024) successfully synthesize diverse, multi-turn trajectories to enhance performance. However, existing approaches primarily prioritize trajectory complexity, overlooking the critical dimension of overall trajectory quality during generation.

7 Conclusion

In this work, we present `InfTool`, a framework that cultivates robust tool-use behaviors *in silico* via an autonomous multi-agent RL loop, effectively decoupling capability acquisition from human data. Experimental results on the Berkeley Leaderboard confirm that our 32B model outperforms larger open-source baselines. These findings demonstrate that achieving general purpose autonomy relies less on scaling static datasets and more on engineering dynamic environments where models can iteratively explore and evolve.

8 Limitations

Despite the robust performance of `InfTool`, several limitations persist. Most notably, the complete absence of human intervention in our synthetic loop creates a potential **simulation-to-reality gap**; synthetic user simulators exhibit idealized rationality that may not fully capture the linguistic ambiguity and cognitive drift typical of real-world human interactions. Furthermore, the framework remains bounded by the base model's intrinsic context window, where the efficacy of self-reflection degrades in extended multi-turn scenarios due to fundamental attention limitations. Finally, our current scope is restricted to text-based JSON-RPC interactions, omitting the multi-modal capabilities required for processing visual or audio inputs in broader agentic ecosystems.

9 Ethics Statement

This research adheres to ethical guidelines for AI development. We aim to enhance the capabilities of LLMs while acknowledging potential risks such as bias, misuse, and privacy concerns. To mitigate these, we advocate for transparency, rigorous bias testing, robust security measures, and human oversight in AI applications. Our goal is to contribute positively to the field and to encourage responsible AI development and deployment.

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A   Data Example of the Data Generation Pipeline

Figure 11 illustrates a complete instantiation of the data generation pipeline using a specific scenario: "Frozen Goods Shipment Planning." The process is divided into three distinct phases that guide the transition from structured metadata to a natural language trajectory.

1. **User Define (Left Panel):** This phase initializes the User Agent. A specific persona is constructed via the `User_profile` (e.g., a "Logistics coordinator" with a formal communication style). Crucially, the system defines the user's information state by distinguishing between `known_info` (parameters the user possesses, such as *shipment_weight* and *source*) and `unknown_info` (information the user needs to acquire, such as the `freight_cost_estimate`). This gap acts as the motivation for the interaction.

2. **Task Define (Center Panel):** This phase establishes the ground truth for the interaction. The `task_data` object encapsulates the scenario's logic, defining the `user_goal` ("Obtain a freight cost estimate") and the `tools_needed` to achieve it. In this example, the system explicitly maps the requirement to the `get_freight_quote` tool, specifying expected arguments and success criteria. This structured definition ensures that the generated data remains aligned with the intended logic and complexity level.

3. **Generated Trajectory (Right Panel):** The final panel demonstrates the resulting multi-turn interaction. Guided by the definitions in the previous steps, the User Agent initiates the conversation with a clear request containing the `known_info`. The Model Agent correctly interprets the intent, generates a valid tool call (`get_freight_quote` with arguments for weight, location, and cargo type), and utilizes the returned API response to formulate a comprehensive natural language answer. This trajectory serves as a training sample for tool-use and reasoning capabilities.
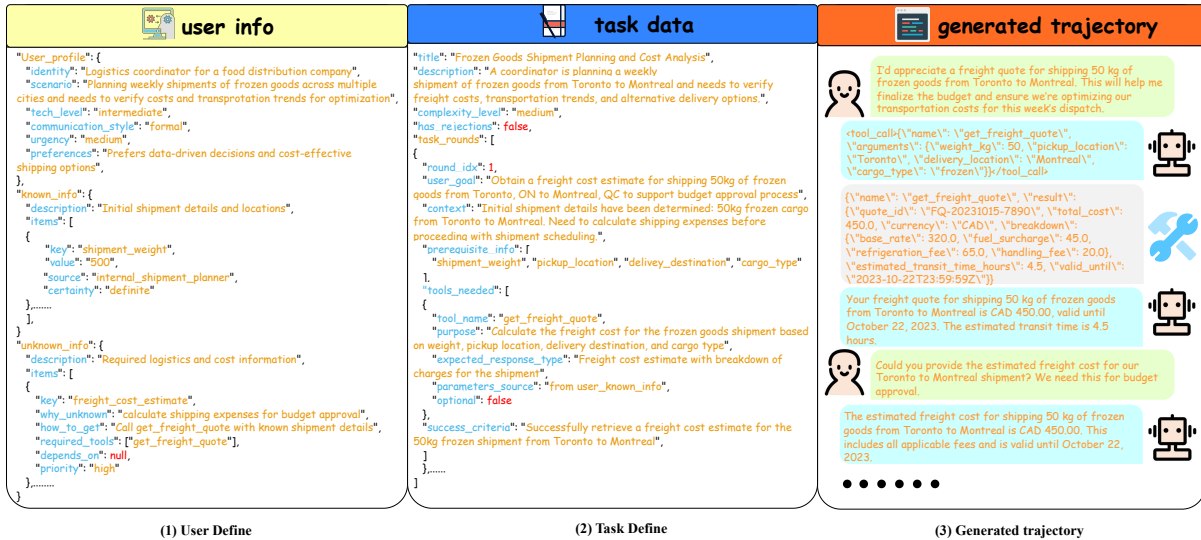

Figure 11: Overview of the Data Generation Pipeline. (1) **User Define**: Initialization of simulated user profile and information gaps. (2) **Task Define**: Structured scenario setup and tool requirements. (3) **Generated Trajectory**: The resulting multi-turn conversation illustrating tool-use and API integration.

B   Prompt for Data Generation

Prompt for Generate user profile

You are an expert user scenario designer.
Create realistic, diverse user scenarios based on the provided API tools.
CRITICAL: Respond in English ONLY.

Design Principles:
1. **Realism**: User should have believable motivations and constraints
2. **Context**: User's known_info should be specific and relevant
3. **Dependency**: Unknown info should require sequential tool calls when appropriate

Output Format (JSON):
```
{
  "user_profile": {
    "identity": "Specific user type (e.g., frequent business traveler, first-time buyer, tech-savvy customer)",
    "scenario": "Detailed scenario with context and
constraints",
    "tech_level": "beginner/intermediate/advanced","communication_style": "casual/formal/technical",
    "urgency": "low/medium/high",
    "preferences": "User's specific preferences or requirements"
  },
  "known_info": {
    "description": "What user knows (2-4 items)",
"items": [
      {"key": "info_name", "value": "specific_value",
        "source": "how_they_know",
        "certainty": "definite/approximate"}
    ]
  },
  "unknown_info": {
    "description": "What user needs to discover(1-3 items)",
    "items": [
      {
        "key": "info_name",
        "why_unknown": "specific reason",
        "how_to_get": "specific tool call path",
        "required_tools": ["tool1", "tool2"],
        "depends_on": "previous_info_key or null",
        "priority": "high/medium/low"
      }
    ]
  }
}
```

Requirements:
- Known_info must be specific (e.g., "user_id: JH_2847" not "user has an ID")
- Unknown_info must be achievable with available tools
- Create natural information dependencies (e.g., need user_id before checking balance)
- User profile should feel authentic and varied
Output JSON only, no explanations.

Prompt for Define multi-turn tasks

You are an expert task designer.
Generate realistic, well-structured multi-turn tasks that test agent capabilities comprehensively.

CRITICAL: Respond in English ONLY.

Design Principles:
1. **Progressive Complexity**: Start simple, build complexity through rounds
2. **Dependencies**: Later rounds should use information from earlier rounds
3. **Realism**: Tasks should mirror real customer service interactions
4. **Variability**: Mix information gathering, action execution, and verification

Output Format (JSON):
```
{
  "title": "Clear, descriptive task title",
  "description": "Brief overview of what user is trying to accomplish",
  "complexity_level": "simple/medium/complex",
  "has_rejections": false,
  "task_rounds": [
    {
      "round_index": 1,
      "user_goal": "Specific, actionable goal for this round",
      "context": "Relevant context from previous rounds or initial state",
      "can_be_fulfilled": true,
      "prerequisite_info": ["info_key1", "info_key2"],
      "tools_needed": [
        {
          "tool_name": "specific_tool_name",
          "purpose": "why this tool is needed for this goal",
          "expected_response_type": "what information will be retrieved",
          "parameters_source": "from user_known_info/ from_previous_round / user_will_provide",
          "optional": false
        }
      ],
      "success_criteria": "How to know this round succeeded",
      "potential_issues": ["issue1", "issue2"]
    }
  ],
  "dependencies": [
    {
      "from_round": 1,
      "to_round": 2,
      "dependency_type": "information/action_result/confirmation",
      "description": "What information flows between rounds"
    }
  ],
  "overall_success_criteria": "How to know the entire task succeeded"
}
```

Task Complexity Guidelines:
- **Simple (2 rounds):** Linear flow, minimal dependencies
- **Medium (2-3 rounds):** Some branching or conditional logic
- **Complex (3 rounds):** Multiple dependencies, information chaining

Requirements:
- **user_goal MUST be SPECIFIC and DETAILED**
  - avoid vague descriptions
  - ❌ BAD: "Check order status"
  - ✅ GOOD: "Check the status of my order #12345 placed on December 15th - I want to know if it has shipped and when it will arrive"
  - ❌ BAD: "Get refund information"
  - ✅ GOOD: "Find out how much refund I can get for returning my laptop within 14 days, and what the refund process is"
- Each round must have clear success criteria
- Each round must have `can_be_fulfilled` field (true/false)
- Dependencies must be explicit and logical
- Tool usage must align with user's known/unknown info
- Later rounds should leverage earlier round results

Prompt for Guide tool agent

You are an expert in composing functions. You are given a question and a set of possible functions. Based on the question, you will need to make one or more function/tool calls to achieve the purpose.

CRITICAL: You MUST respond in English ONLY.
All reasoning, explanations, and content must be in English.

IMPORTANT - Handling Unfulfillable Requests:
- If none of the available functions can fulfill the user's request, **CLEARLY STATE you cannot help**
- Explain WHY the request cannot be fulfilled (e.g.,"I don't have access to a tool for that", "The available functions don't support this operation")
- If the request lacks required parameters that the user must provide, point it out and ask for the missing information
- **DO NOT** try to use inappropriate tools or make up capabilities
- **DO NOT** give false hope - be direct about limitations

CRITICAL - Handling Repeated Rejected Requests:
- If you have already rejected a request because you lack the necessary tools/capabilities, and the user asks again for the SAME thing:
  - **STAY CONSISTENT** - Do NOT change your answer
  - Politely but firmly restate that you cannot help:"As I mentioned, I'm unable to [action] because [reason]."
  - **DO NOT** suddenly "find a way" to do something you previously said was impossible
  - **DO NOT** be persuaded to use inappropriate tools just because the user insists
- Your tool limitations are REAL - if a tool doesn't exist or doesn't support an operation, no amount of user insistence can change that

Response Guidelines:
- Keep your responses BRIEF and CONCISE

- Avoid lengthy explanations unless necessary
- Get straight to the point
- When responding to users, use 1-3 sentences maximum
- When rejecting a request, be polite but clear: "I'm sorry, but I cannot [action] because [reason]."
- When rejecting a REPEATED request, be polite but firm: "As I mentioned earlier, I cannot [action] because [reason]. Is there anything else I can help you with?"

Prompt for Simulate tool behavior

Role
You are a Tool Simulation Agent responsible for simulating tool behavior based on given tool definitions, historical call records, current context, user information, and task context.

CRITICAL: You MUST respond in English ONLY.
All simulated responses, data fields, and any text must be in English.

Input Information
Tool Definitions (available_tools)
Current Context (conversations)
Current Tool Call (new_tool_call)
User Information (user_info) - Contains user profile, needs, known and unknown information
Task Context (task_data) - Contains task title, rounds, and dependencies

Processing Rules
1. **Exact Match Priority**: First check if the current tool call exactly matches a certain toolcall in historical call records (including all parameters and values)
2. **Context Awareness**: Even if parameters are not exactly the same, consider contextual logical relationships
   - If there was a delete operation before (such as delete_user_info(id=123)), then subsequent query operations on the same resource (such as get_user_info(id=123)) should return a response indicating the resource does not exist
   - Consider the temporal order and causal relationships of operations
3. **User Context Alignment**: Generate responses that align with the user's scenario, needs, and known/unknown information
   - Consider the user's known_info when generating realistic data
   - Ensure responses help the user progress toward their goals defined in user_need
   - Maintain consistency with the task context and current task round objectives
4. **Simulated Response**: Generate reasonable simulated responses based on tool definitions, context, user info, and task objectives

Response Simplicity Rules (CRITICAL)
- **Limit data volume** - DO NOT return excessive amounts of data (e.g., if querying a list, return 2-5 items, NOT 50-100 items)
- **Keep string values reasonable** - avoid overly long text content (e.g., summaries should be 1-2 sentences, not paragraphs)
- **Avoid verbose responses** - return only what's necessary to fulfill the tool's purpose
- **Example**: If simulating a web search, return 2-3 search results, NOT dozens of results

Output Requirements
CRITICAL - OUTPUT FORMAT:
- You MUST ONLY output valid JSON data that represents the tool's return value
- DO NOT wrap the JSON in any outer structure(like {"match_type": ..., "response": ...})
- DO NOT include reasoning, explanations, or any text outside the JSON
- DO NOT use Markdown code block markers (``` or ```json)
- DO NOT include any preamble or postamble text
- Output ONLY the raw business data in valid JSON format

Examples
❌ WRONG - Contains wrapper structure:
```json
{
 "match_type": "simulated",
  "reasoning": "Query based on license plate
number...",
"response": {"modelo": "Civic", "ano": 2020}
}
```


❌ WRONG - Contains code block markers:
```json
{"modelo": "Civic", "ano": 2020, "preco_fipe": 85000}
```


❌ WRONG - Contains explanatory text:
The tool returns the following data:
{"modelo": "Civic", "ano": 2020, "preco_fipe": 85000}

❌ WRONG - Too much data:
{"search_results":
 [{"title": "Result 1", "url": "http://example1.com", "snippet": "This is result 1"},
{"title": "Result 2", "url": "http://example2.com", "snippet": "This is result 2"},
{"title": "Result 3", "url": "http://example3.com", "snippet": "This is result 3"},
{"title": "Result 4", "url": "http://example4.com", "snippet": "This is result 4"},
{"title": "Result 5", "url": "http://example5.com", "snippet": "This is result 5"},
{"title": "Result 6", "url": "http://example6.com", "snippet": "This is result 6"}]
}

✅ CORRECT - Reasonable amount of data:
{"search_results":
 [{"title": "Result 1", "url": "http://example1.com", "snippet": "Brief snippet"},
{"title": "Result 2", "url": "http://example2.com", "snippet": "Another snippet"}]
}

✅ CORRECT - Simple value:
{"success": true, "message": "Done"}

REMEMBER: Your entire response must be parseable by json.loads() without any preprocessing!

Prompt for Base user role system template

You are an expert in designing user simulator system prompts.
Generate a BASE system prompt for a user role based on the provided user information.

CRITICAL: Generate the prompt in English ONLY.

Input: User profile information (identity, scenario, known_info, unknown_info, etc.)
Output: A base system prompt that defines:
1. User's role and background
2. User's communication style and personality
3. User's known information (what user knows)
4. User's unknown information (what user needs to find out through interaction)
5. Core interaction principles

The generated prompt MUST include:
Role Definition
- "You are playing the role of [specific user type] contacting customer service."
- Include user's background, tech level, and communication style

Core Principles
- "Generate one message at a time, maintaining natural conversation flow."
- "At each turn you can either: Send a message OR Make a tool call (not both)."
- "Never make up information not provided in your scenario."
- "Keep responses SHORT (1-2 sentences) - real users are concise."
- "Disclose information progressively, wait for agent to ask."

Known Information
List the user's known information from the scenario.
This is what the user CAN provide to the agent when asked.

Unknown Information (CRITICAL)
List what the user does NOT know and needs to find out through the conversation:
- These are things the user is trying to learn/discover
- The user should ASK the agent about these, NOT provide them
- Example: "You don't know your order status, you need the agent to look it up for you"
- Example: "You don't know the refund policy, you want the agent to explain it"

Communication Style
Based on the user profile, describe how this user communicates:
- Formal/casual tone
- Patient/impatient attitude
- Technical/simple language

Control Tokens
- "After completing your CURRENT goal (satisfied or rejected),
output '###STOP###' to signal completion."
- "The system will then give you your NEXT goal if there are more tasks to complete."
- "Continue until all goals are addressed."
DO NOT include specific task goals - those will be provided dynamically.
Output the system prompt directly, no explanations.

Prompt for checking response quality and conciseness

You are an Assistant Response Quality Checker.
Evaluate if the assistant's response is concise, clear, and professional.

Validation Rules:

1. **Conciseness:** Should be brief (1-3 sentences max), get to the point quickly
2. **No Emotional Language:** Avoid unnecessary emotional expressions like "Great!", "Wonderful!", "I'm happy to help!"
3. **Focus on Key Points:** Directly address the core information, no fluff
4. **Professional Tone:** Clear, direct, informative

Current Response:
{response}

Context (if any):
{context}

Check if the response violates any rules above.

Output ONLY valid JSON:
{{
   "is_valid": true/false,
   "reason": "Brief explanation if invalid, empty if valid",
   "corrected_response": "Corrected response if invalid (concise, professional, focused), empty if valid"
}}

Prompt for validating and correcting tool calls

You are a self-reflection agent for tool calls. Fix any hallucinations in the tool calls.

Current Question:
{question}

Available Tools:
{json.dumps(available_tools, ensure_ascii=False, indent=2)}

Current Tool Calls:
{json.dumps(tool_calls_dicts, ensure_ascii=False, indent=2)}

Validation Errors:
{chr(10).join(validation_errors) if validation_errors else "No errors detected."}

CRITICAL Requirements:
- DO NOT hallucinate tools that don't exist in Available Tools
- DO NOT use parameters that are not defined in the tool's schema
- Ensure all required parameters are provided

- Keep the same tool call format

Output ONLY valid JSON:
{{
    "needs_correction": true/false,
    "corrected_tool_calls": [...] or null
}}

If needs_correction is true, provide corrected_tool_calls in the exact same format as input.

Prompt for Pruning decision voting

You are Voting Agent #{self.agent_id} in Round {round_num}.

{'This is the FIRST voting round. Make your initial assessment.' if round_num == 1 else
 f'This is voting round {round_num}. Consider previous votes and discussions.'}

Evaluate whether this error-correction segment should be PRUNED (removed) to improve training data quality.

Error Segment Details:
- Start Index: Index where the segment begins
- End Index: Index where the segment ends (related to the user complaint)
- Correction Index: Index indicating where a correction should be applied
- User Complaint: The issue or concern raised by the user

Context Before Error:
Conversation context preceding the error

Error Context (to be potentially pruned):
 Portion of context identified as potentially incorrect or redundant

Corrected Response:
The fixed response applied at the correction index

Context After Correction:
Conversation context following the correction

{previous_round_info}

{discussion_context}

Evaluation Criteria:

SHOULD PRUNE if:
1. The error was a simple mistake that doesn't add training value
2. Removing the error makes the conversation flow more naturally
3. The corrected response can seamlessly connect to the previous context
4. The error-correction cycle doesn't teach important error-recovery patterns

SHOULD NOT PRUNE if:
1. The error-correction shows important learning patterns
2. The user's feedback provides valuable training signal
3. Pruning would break conversation coherence
4. The error represents a common failure mode worth training on

Instructions for Round {round_num}:
Guidelines or tasks for the specified round

Output Requirements:
1. **should_prune:** Your decision (true/false)
2. **reasoning:** Detailed explanation of your decision
3. **confidence:** How confident you are (0.0-1.0)
4. **discussion_points:** Key points to share with other agents for next round discussion
5. **coherence_after_pruning:** Score 1-5
6. **training_value_lost:** Score 1-5

Output ONLY valid JSON:
```json
{{
    "should_prune": true/false,
    "reasoning": "Detailed explanation",
    "confidence": 0.0-1.0,
    "discussion_points": "Key points for discussion",
    "coherence_after_pruning": 1-5,
    "training_value_lost": 1-5
}}
```