# Towards Reliable and Scalable Autonomous Agents: Bridging the Gap for Tool-Use in Real-World Agentic Tasks

*Xingshan Zeng*

*Huawei HKRC*



# Bio

- **Name:** ZENG, Xingshan (曾幸山)
- **Research Interests:** NLP, LLM Agents, Evaluation & Reasoning
- **Working Experience:**
  - 2020 – Now: Senior Researcher at Huawei Hong Kong Research Center
- **Education Experience:**
  - 2016 – 2020: Ph.D. at CUHK SEEM
  - 2012 – 2016: B.Eng. at USTC CST
- Published **more than 40 papers** on top conferences and journals, **18** of them are as first-author/corresponding author. Google scholar citation **2200+**.
- Led the development of the **ToolACE series**, whose models ranked **#1** on BFCL and have accumulated **over 600K** downloads.
  - Core agentic techniques integrated into Huawei Pangu models
  - Deployed in products across Huawei Devices and Cloud Services
- M4LE (mentoring intern work) won ACL24 **Outstanding Paper** Award.

# Outline

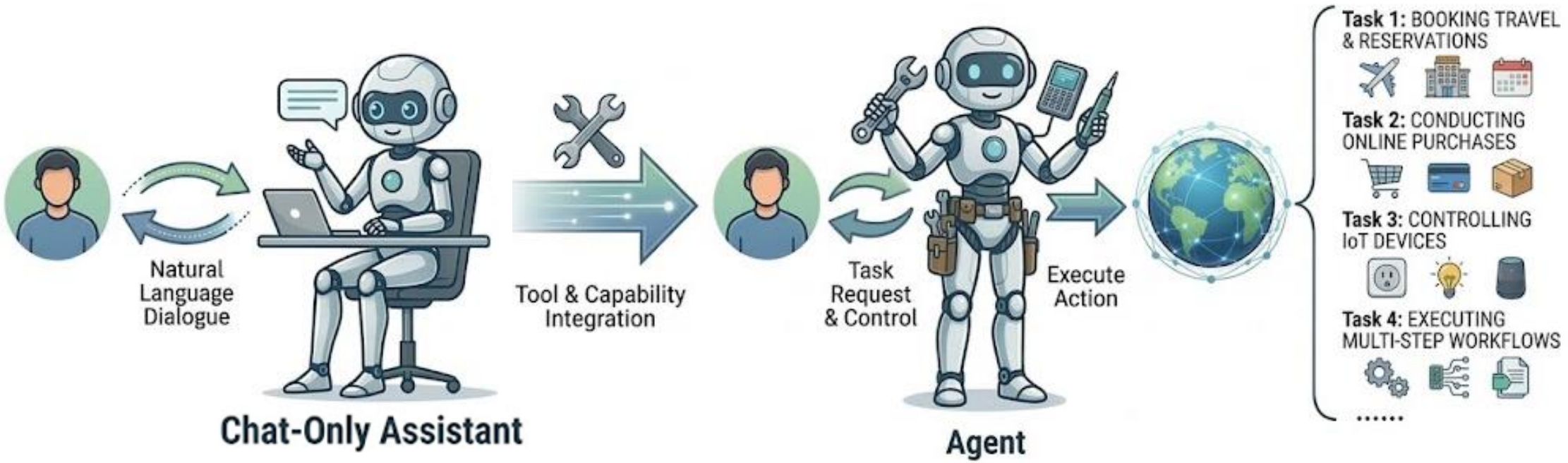
- Overview of LLM-based Agents
- Scaling Capability: Scalable Agentic Data Generation
- Improving Potential: Model-Aware Training and Inference Scaling
- Summary and Future Horizons: Towards Next-Generation Agents

# Outline

- **Overview of LLM-based Agents**
- Scaling Capability: Scalable Agentic Data Generation
- Improving Potential: Model-Aware Training and Inference Scaling
- Summary and Future Horizons: Towards Next-Generation Agents

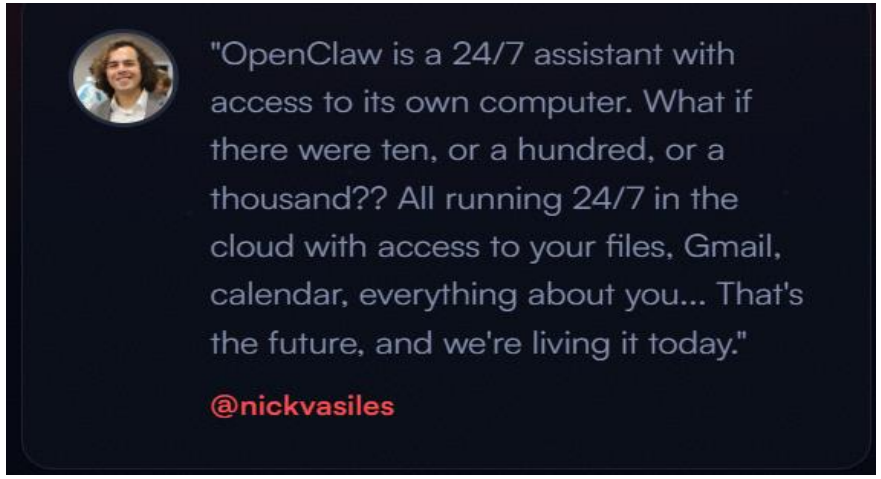
# What are LLM-based Agents?

- **LLMs Acting as Brain:** For perception, planning, and decision-making
- **Real-World Interaction:** Access to external environment (through **tools**)
- From chat-only assistant to a more powerful **task solver**



# What Can LLM-based Agents Do?




**OpenClaw: Personal Assistant**




**Claude Code: Coding Agent**







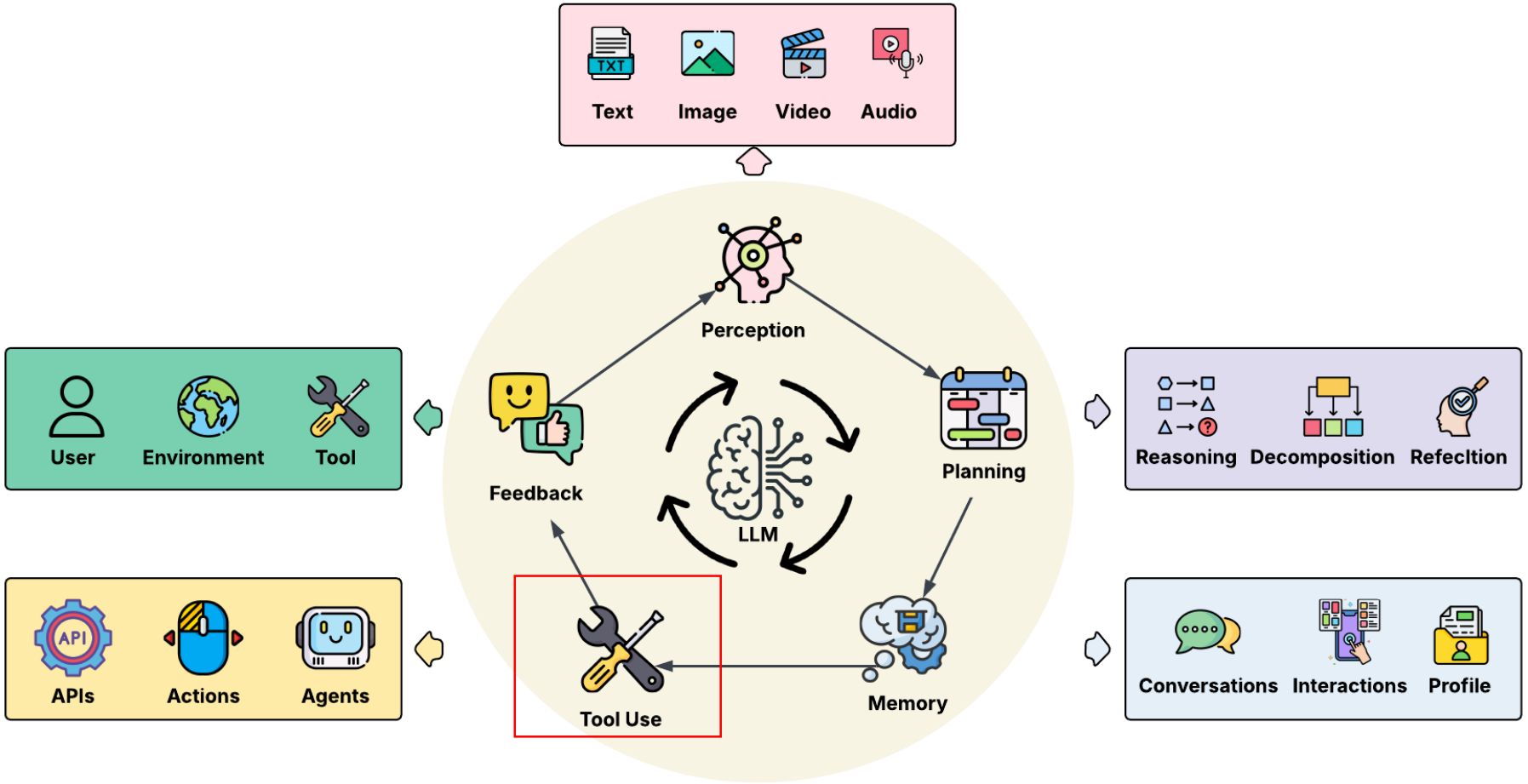


**Deployed in Car, Phone, etc.**

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# Key Capabilities of LLM-based Agents

- **Tool Use**: Capability to handle diverse tools and use them correctly



# How Do Current Agents Perform?

| Model | Normal | Special | Agent | Overall |
|---|---|---|---|---|
| GPT-4o | 87.6 | 93.0 | 63.8 | **85.4** |
| Gemini-2.5-Pro-05-06 | 80.7 | 90.0 | 63.8 | **80.6** |
| Qwen-Max | 84.2 | 74.0 | 64.3 | **78.4** |
| GPT-4o-Mini | 79.9 | 79.0 | 33.3 | **72.5** |
| Gemini-1.5-Pro | 79.0 | 78.7 | 25.5 | **70.7** |
| Claude-3-5-Sonnet | 72.9 | 77.4 | 39.5 | **68.9** |
| Doubao-Pro-32K | 70.7 | 55.0 | 25.0 | **59.4** |

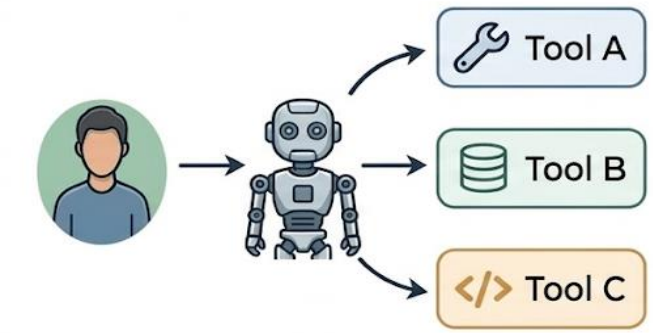
- **Evaluation Scenarios (ACEBench):**
  - **Normal:** Single-Turn with diverse parameter types **(Basic Tool Use)**
  - **Special:** Handling abnormal requirements **(Non Tool Use)**
  - **Agent:** End-to-end handling for complex user tasks **(Complex Tool Use)**

**Agents still Struggle with Complex Tool Use!**

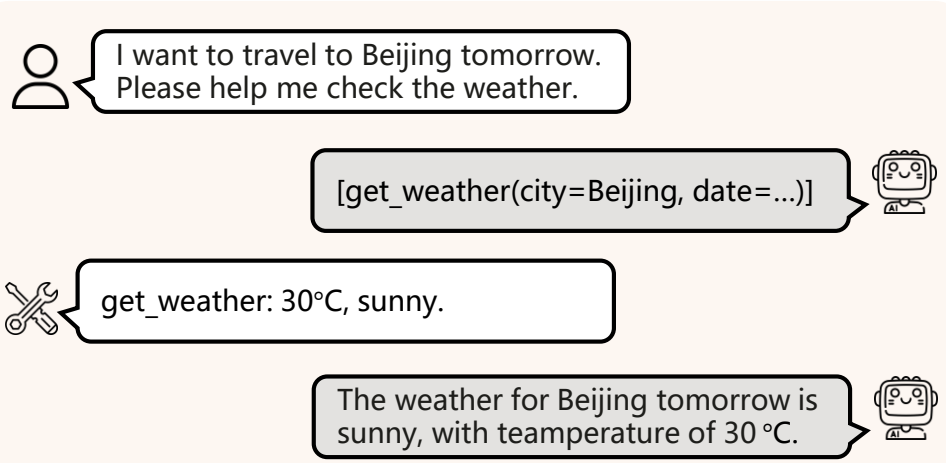


Chen Chen, et al. "ACEBench: A Comprehensive Evaluation of LLM Tool Usage." *EMNLP 2025 Findings.*

# Basic Tool Use vs. Complex Tool Use

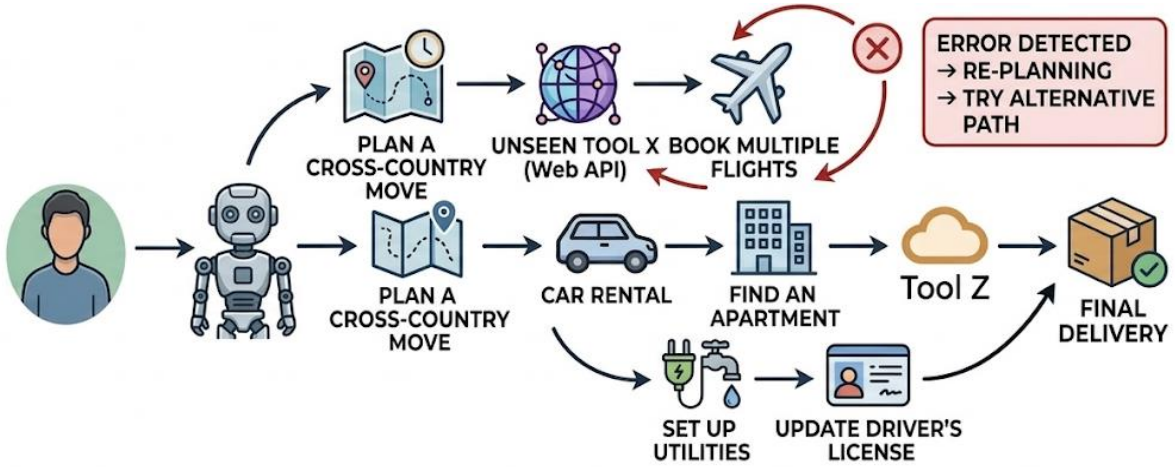



**Basic Tool Use**

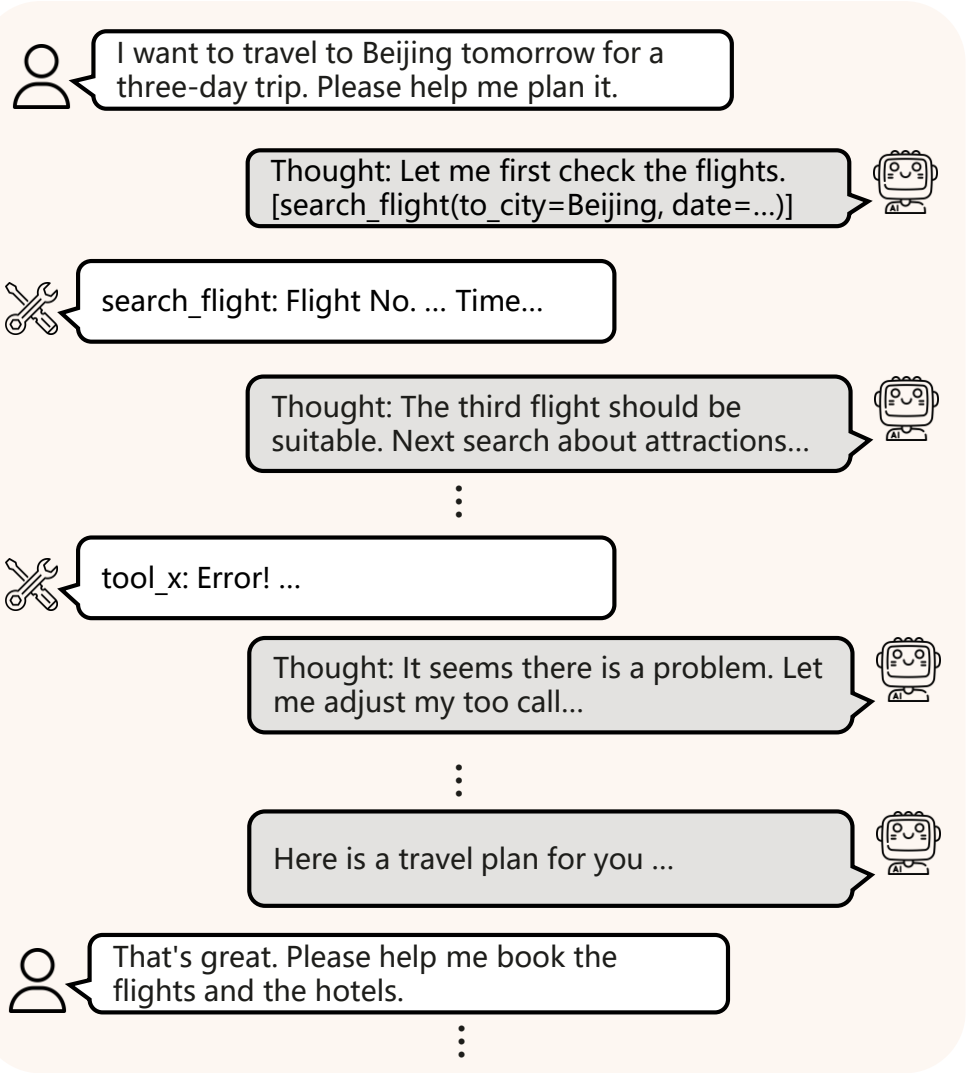



- **Basic Tool Use:**
  - **Explicit Requirement:** The user query is generally clear
  - **Single-Turn:** One single query from the user
  - **Single-Step:** One single tool calling can solve the problem

# Basic Tool Use vs. Complex Tool Use




**Complex Tool Use**

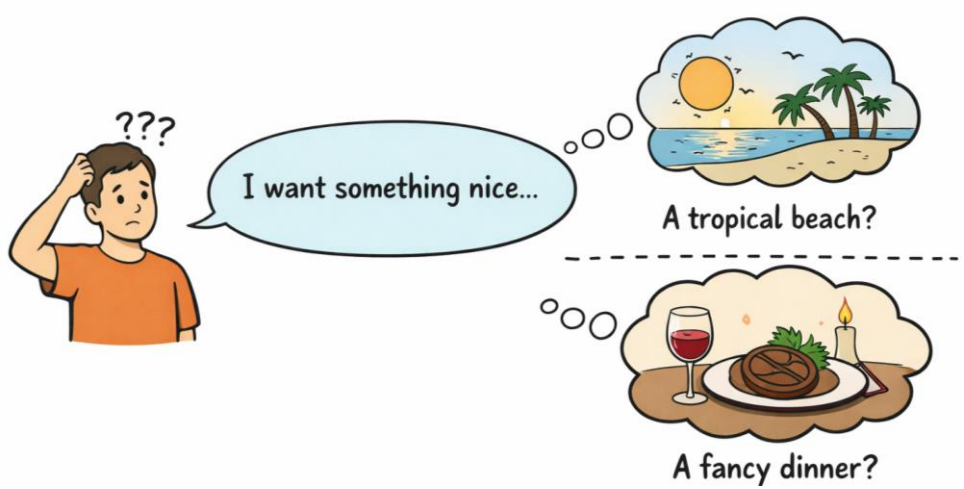



- **Complex Tool Use:**
  - **Long Horizon:** multi-turn, multi-step
  - **Open World:** vast and dynamic tools
  - **Vague User Requests:** need clarification
  - **Error Recovery:** detect failures and adjust

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# Real-World Tasks are Often Complex

- **Human Nature:**
  - **Ambiguous intentions:** Users often provide vague or underspecified requests
  - **Subjective decisions:** Multiple acceptable solutions
- **Environmental Instability:**
  - **Uncertain outcomes:** Tool execution may fail or return noisy results
  - **Partially observable:** The full environment state is usually invisible to agents




**Complex Tool Use is a Key Bottleneck for Building Real-World Agents!**

# Key Challenges for Complex Tool Use

- **Data Gap**
  - Lack of high-quality data

| Model | #API | #Domain | Nested | Parallel | Dependent | Multi-type |
|---|---|---|---|---|---|---|
| Gorilla [14] | 1645 | 3 | ✗ | ✗ | ✗ | ✗ |
| ToolAlpaca [19] | 3938 | 50 | ✗ | ✗ | ✗ | ✗ |
| ToolLLM [15] | 16464 | 49 | ✗ | ✗ | ✓ | ✗ |
| Functionary [12] | n/a | n/a | ✗ | ✓ | ✗ | ✗ |
| xLAM [11] | 3673 | 21 | ✗ | ✓ | ✗ | ✗ |
| Granite [1] | n/a | n/a | ✗ | ✓ | ✗ | ✓ |
| **ToolACE** | **26507** | **390** | ✓ | ✓ | ✓ | ✓ |

- **Data Utilization**
  - How to best leverage the limited data?

- **Inference Reliability:**
  - Balance between Effectiveness and Efficiency

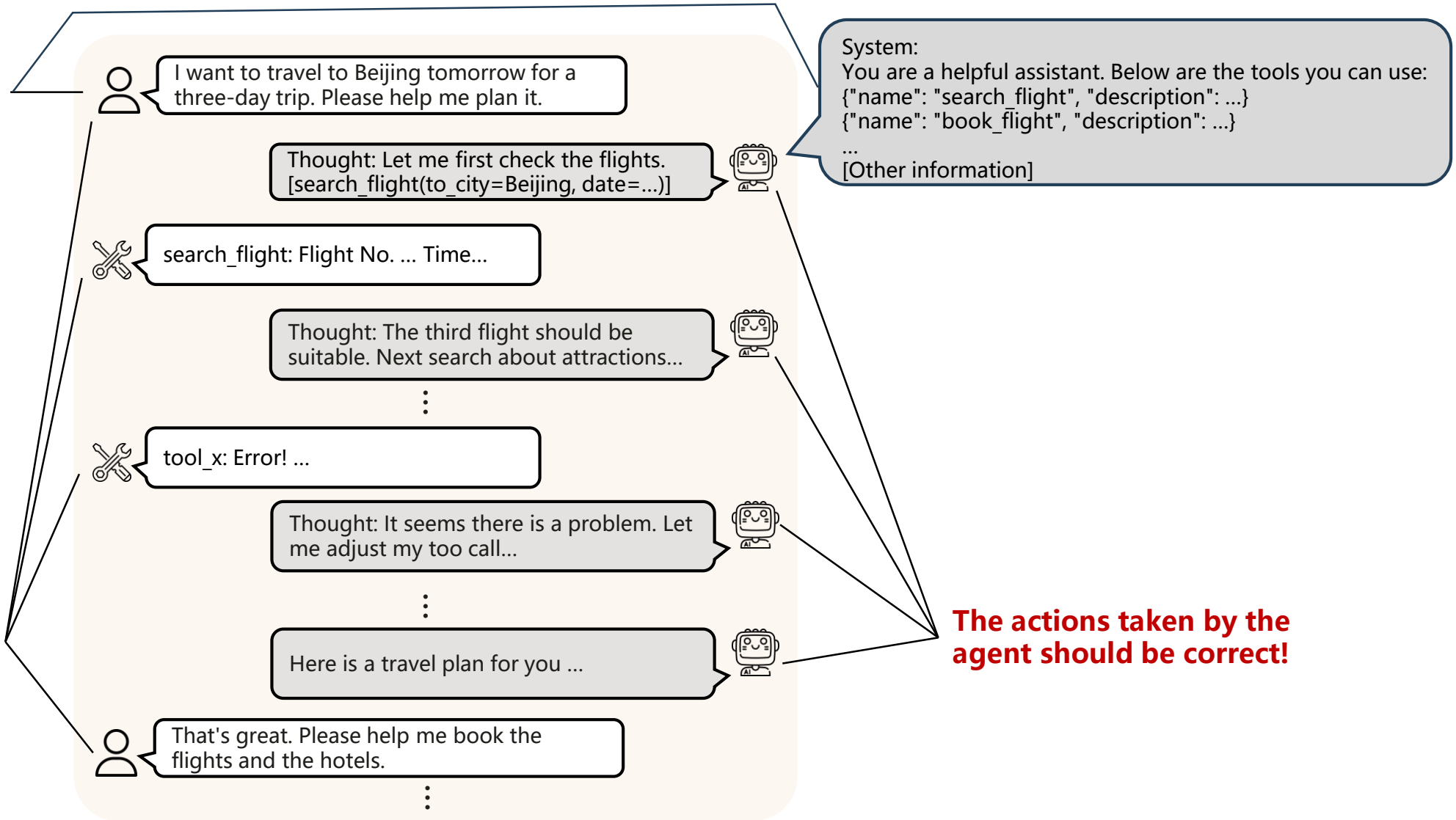


# Outline

- Overview of LLM-based Agents
- **Scaling Capability: Scalable Agentic Data Generation**
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# What Should High-Quality Data Look Like?

**Cover a wide range of scenarios to enable generalization to unseen situations!**



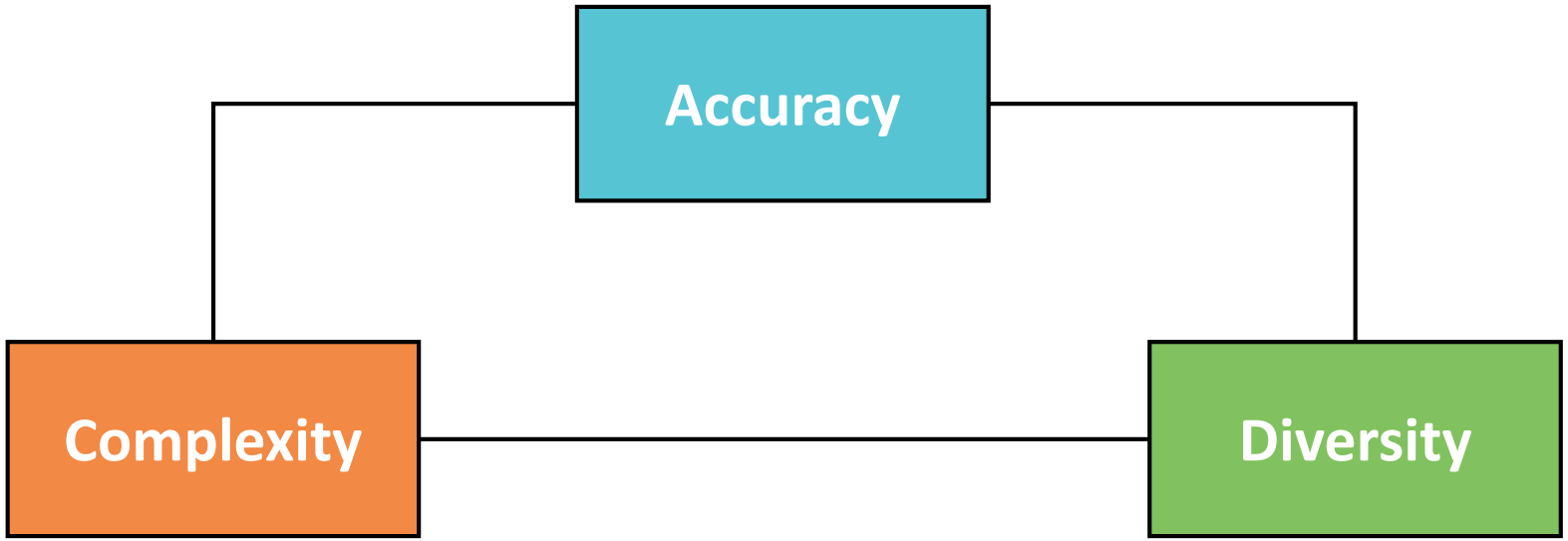

**Approximate the real scenarios (complex)!**

**The actions taken by the agent should be correct!**

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# ToolACE: Accuracy, Complexity, and Diversity

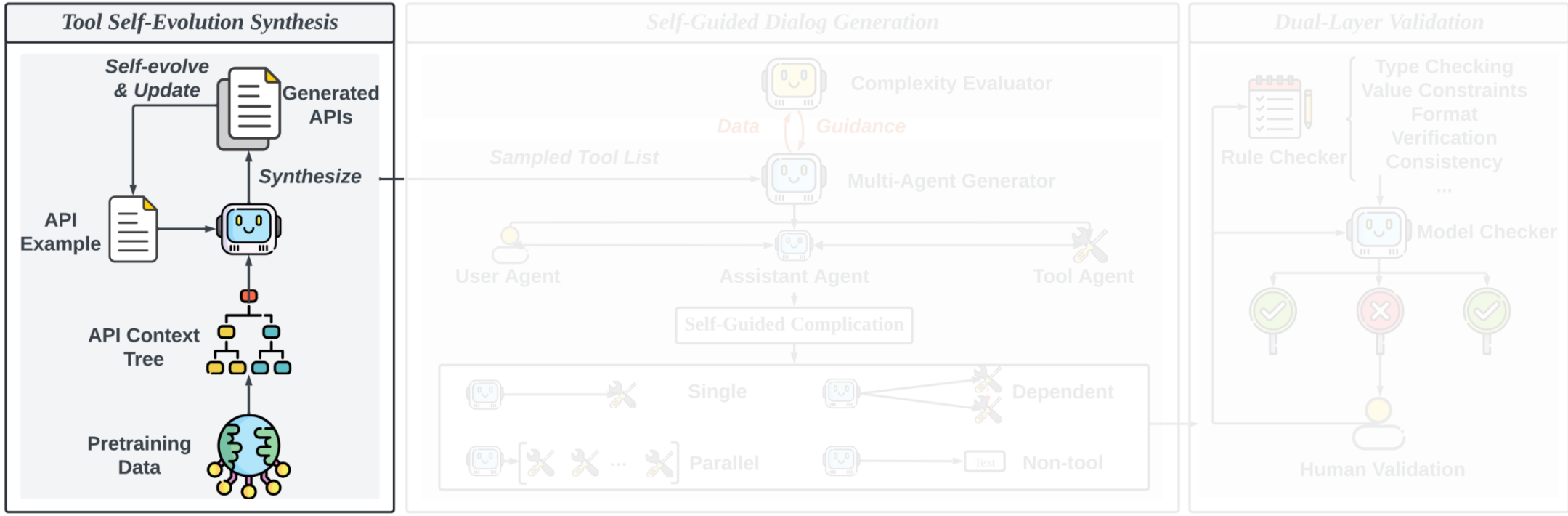
- **Accuracy: Fundamental** to the effectiveness of LLM-based agents; Reduce hallucinations, problematic invocations.
- **Complexity:** Training data should possess sufficient complexity to foster agentic skills; LLMs learn more effectively when the complexity of the data aligns with (**slightly exceeds**) their current capability.
- **Diversity:** Broad range of agentic scenarios enhances their proficiency and zero-shot tool usage; Essential for **out-of-distribution** generalization.






Weiwen Liu*, Xu Huang*, Xingshan Zeng*, et al. "ToolACE: Winning the Points of LLM Function Calling." *ICLR 2025.*

# ToolACE: Agentic Data Generation Framework




**Tool Synthesis**

- Construct API context tree
- Instruct the agent to **iteratively refine and update** the API definitions

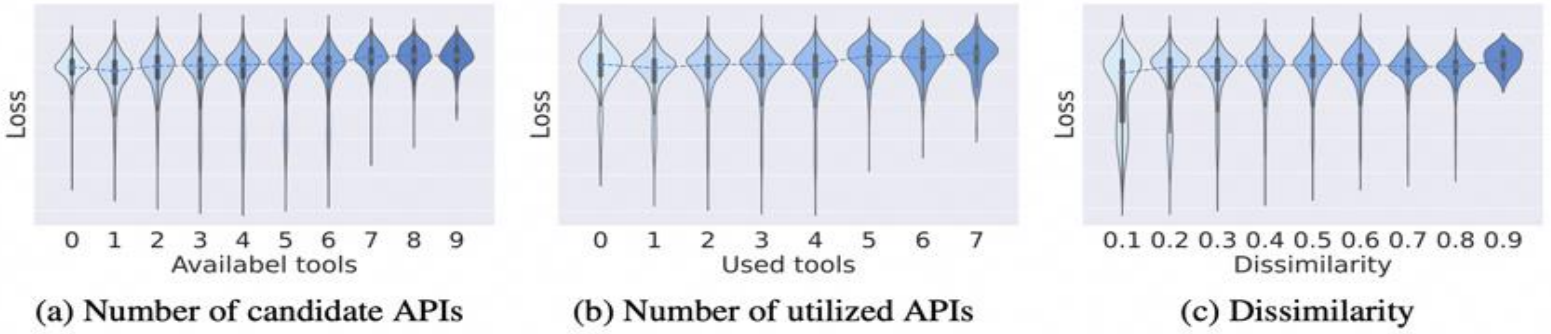
**(Diversity)**

# ToolACE: Agentic Data Generation Framework

➢ **Data Complexity:**

$$H_{\mathcal{M}}(x, y) = -\frac{1}{n_y} \sum_{i=1}^{n_y} \log p(t_i | x, t_1, \ldots, t_{i-1})$$

➢ **Positively correlated** with several signals related to task complexity.




**Tool Synthesis**

- Construct API context tree
- Instruct the agent to **iteratively refine and update** the API definitions

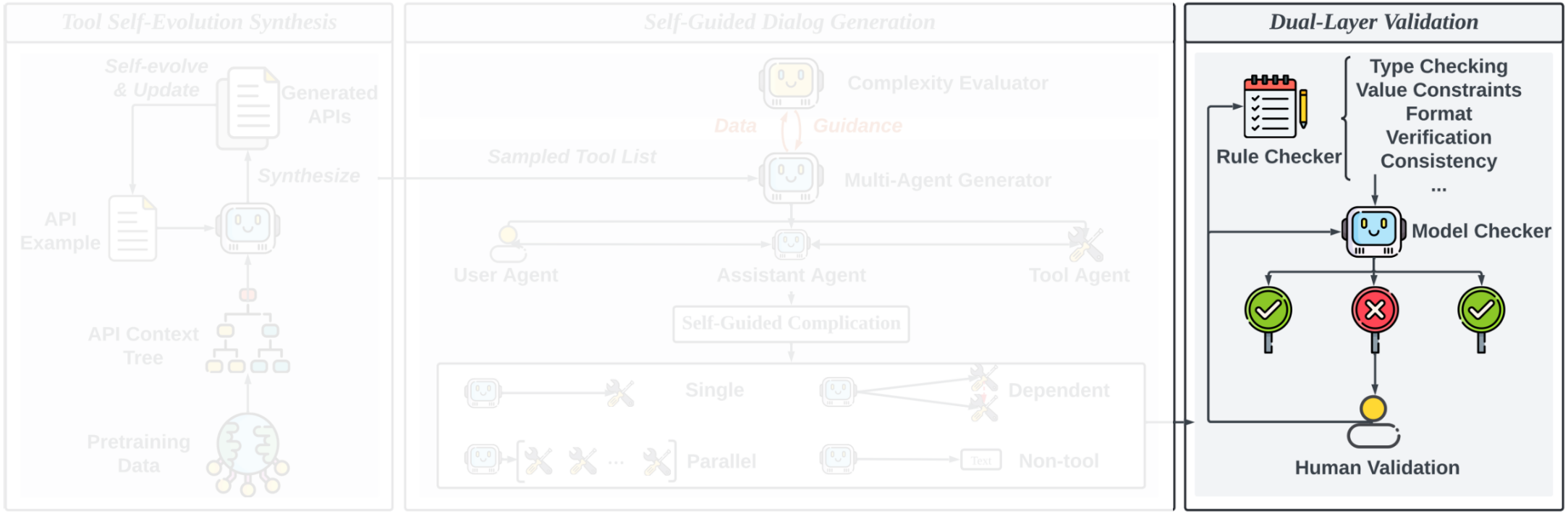
**(Diversity)**

**Dialog Generation**

- **Multi-Agent Simulation**
- Multiple types of dialogs with **Self-Guided Complication**

**(Complexity)**

# ToolACE: Agentic Data Generation Framework




**Tool Synthesis**
- Construct API context tree
- Instruct the agent to **iteratively refine and update** the API definitions

**(Diversity)**

**Dialog Generation**
- **Multi-Agent Simulation**
- Multiple types of dialogs with **Self-Guided Complication**

**(Complexity)**

**Data Verification**
- Rule checker
- Model checker

**(Accuracy)**

# ToolACE: Performance

- **Experiment Setup:** Based on Llama3.1-8B-Instruct, trained with over 200k data.
- **Results:** Competitive to GPT-4o

| Rank | Overall | Model | Single turn | | | Multi turn | Hallucination | |
|---|---|---|---|---|---|---|---|---|
| | | | Non-live (A) | Non-live (E) | Live (A) | Multi turn | Rel | Irrel |
| 1 | 59.49 | GPT-4-turbo-2024-04-09 (FC) | 82.65 | 83.80 | 73.39 | 21.62 | 70.73 | 79.79 |
| 2 | 59.29 | GPT-4o-2024-08-06 (FC) | 85.52 | 82.96 | 71.79 | 21.25 | 63.41 | 82.91 |
| 3 | 59.22 | ToolACE-8B (FC) | 89.27 | 90.07 | 73.21 | 14.37 | 85.37 | 83.81 |
| 4 | 59.13 | xLAM-8x22b-r (FC) | 89.75 | 89.32 | 72.81 | 15.62 | 97.56 | 75.23 |
| 5 | 58.45 | GPT-4o-mini-2024-07-18 (FC) | 82.83 | 81.80 | 67.53 | 25.75 | 82.93 | 71.83 |
| 6 | 57.94 | xLAM-8x7b-r (FC) | 88.44 | 85.89 | 71.97 | 15.75 | 92.68 | 72.35 |
| 7 | 57.21 | GPT-4o-mini-2024-07-18 (Prompt) | 86.54 | 87.95 | 72.77 | 11.62 | 80.49 | 79.20 |
| 8 | 55.82 | mistral-large-2407 (FC) | 84.12 | 83.09 | 67.17 | 20.50 | 78.05 | 48.93 |
| 9 | 55.67 | GPT-4-turbo-2024-04-09 (Prompt) | 91.31 | 88.12 | 67.97 | 10.62 | 82.93 | 61.82 |
| 10 | 54.83 | Claude-3.5-Sonnet-20240620 (FC) | 70.35 | 66.34 | 71.39 | 23.50 | 63.41 | 75.91 |

Results on BFCL

# ToolACE: Effects of "ACE"

- **Accuracy** highly correlates with the performance.
- **Medium complexity** performs the best!
- **High diversity** helps (but mild).




Figure 3: Ablation study of the dual-layer verification(DLV).

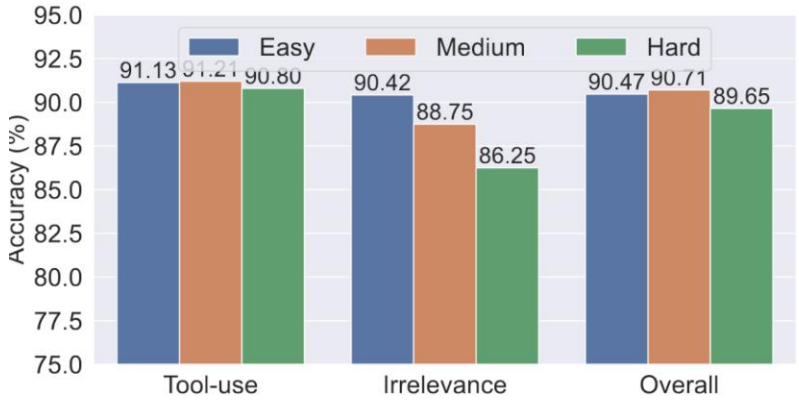



Figure 4: Ablation study on complexity.

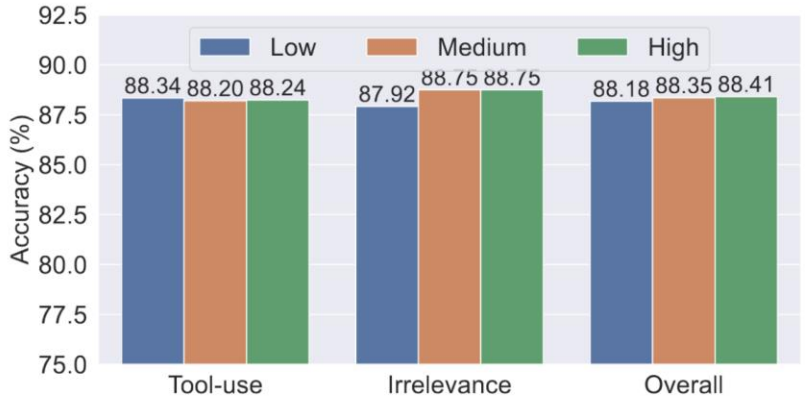
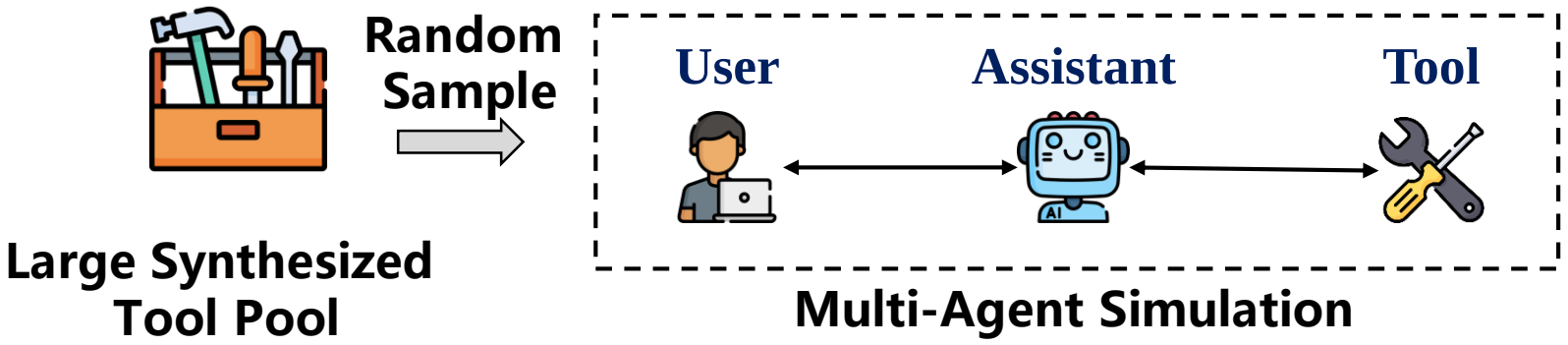



Figure 5: Ablation study on diversity.

# Towards Better Data Generation

- **ToolACE provides a scalable foundation:**

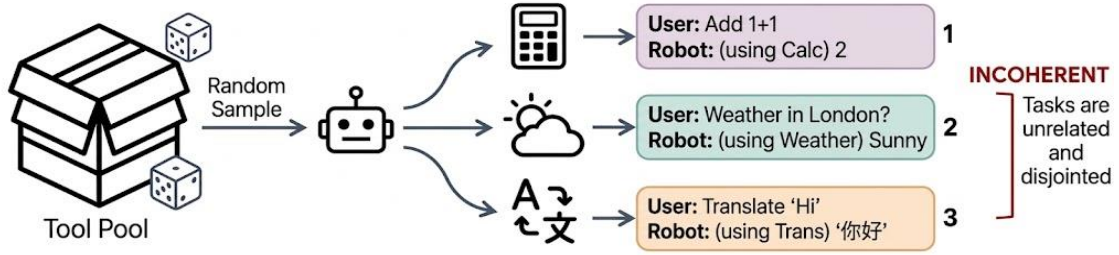



**But it still has limitations!**

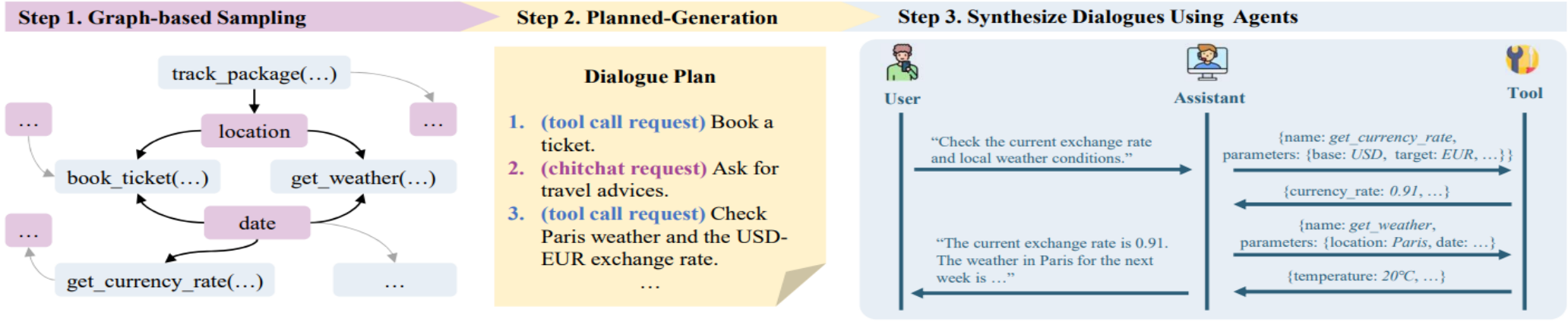
- **Limitation 1:**
  - The candidate tools are more likely to be **unrelated**
  - Possible results: **Unnatural** task synthesis
- **Limitation 2:**
  - Long horizon tasks require extensive LLM calls to form final trajectory (**Costly**)
  - Simulation once begin, it is difficult to alter or interrupt (**Uncontrollable**)

# ToolFlow: Natural and Coherent Synthesis

- **Limitation: "Semantic Isolation" → Unrelated and Disjointed Tasks!**




- **Our Solution: ToolFlow**
  - **Graph-based Sampling:** producing connected candidate tools for related task generation
  - **Planned Generation:** guiding the dialogue development to ensure dialogue coherence






Zezhong Wang, Xingshan Zeng#, et al. "ToolFlow: Boosting LLM Tool-Calling Through Natural and Coherent Dialogue Synthesis." *NAACL 2025.*

# ToolFlow: Graph-based Sampling

- **Tool Graph Construction:**
  - Directional Graph with tools as nodes, connections as edges
  - Edges definition base on: **P-P Similarity** + **P-R Similarity**

$$e_{i,j} = \begin{cases} 1, & \exists p_k^i \subseteq v_i, p_l^j \subseteq v_j : \cos(\mathbf{p}_k^i, \mathbf{p}_l^j) > \tau \\ & \text{or} \\ & \exists r_k^i \subseteq v_i, p_l^j \subseteq v_j : \cos(\mathbf{r}_k^i, \mathbf{p}_l^j) > \tau \\ 0, & \text{otherwise} \end{cases}$$

- **Tool Sampling:**
  - **Random walk** on the graph
  - Initializing from a random node


```
{
  "name": "weather_search",
  "description": "Search for weather information",
  "arguments": {"type": "object", "properties": {
    "city": {"description": "The city name to search for","type": "string"},
    "date": {"description": "The date for the weather search (format: YYYY-MM-DD)","type":
"string","pattern": "\d{4}-\d{2}-\d{2}"}},"required": ["city","date"]}}
  "results": {"type": "object", "properties": {
    "weather": {"description": "Weather details and conditions","type": "string"},
    ...}
}
```

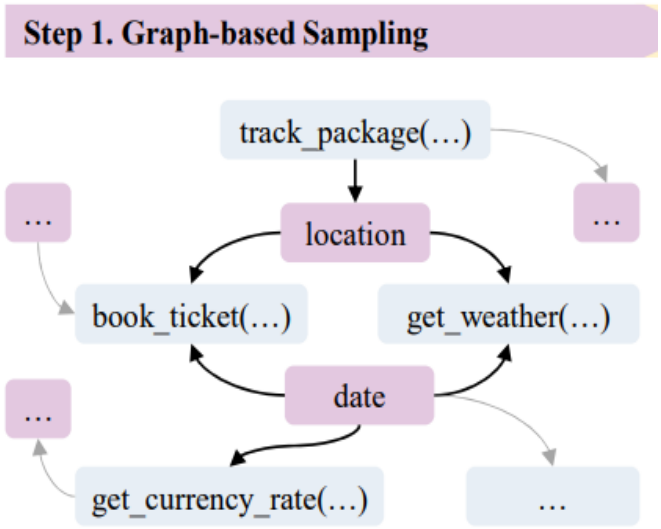

A Tool Example

**Algorithm 1** Graph-based Sampling

**Require:** $G = (V, E)$ with $|V| = N$, integer $n \leq N$ (desired sample size)
**Ensure:** Subset $\hat{V} \subseteq V$ with $|\hat{V}| = n$

*// Randomly choose a node from $V$ and add it to $\hat{V}$*
$\hat{V} \leftarrow \{\text{Uniform}(V)\}$
**while** $|\hat{V}| < n$ **do**
  $v_i \leftarrow$ last element of $\hat{V}$
  *// Find all neighbors of $v_i$*
  $N(v_i) \leftarrow \{v_j \in V \mid e_{i,j} = 1, \forall e_{i,j} \in E\}$
  *// Randomly choose a neighbor of $v_i$*
  $v_j \leftarrow \text{Uniform}(N(v_i))$
  **if** $v_j \notin \hat{V}$ **then**
    *// Add $v_j$ to $\hat{V}$ if not already included*
    $\hat{V} \leftarrow \hat{V} \cup \{v_j\}$
  **end if**
**end while**
**return** $\hat{V}$

Algorithm for Tool Sampling




A Graph Snippet




Zezhong Wang, Xingshan Zeng#, et al. "ToolFlow: Boosting LLM Tool-Calling Through Natural and Coherent Dialogue Synthesis." *NAACL 2025.*

# ToolFlow: Improved Data Quality

- **Graph Sampling → Diversity**
- **Planned Generation → Coherence**
- **Graph + Plan** achieves considerable improvement with only 8K instances

| Automatic Evaluation | | | | | |
|---|---|---|---|---|---|
| *Setting* | | *Coherence* | | *Diversity* | |
| *Graph* | *Plan* | *SS* | *EnR* | *H* | *D-3* |
| ✓ | ✓ | 63.36 | 47.3 | 10.36 | 0.4865 |
| ✓ | ✗ | 62.03 | 32.1 | 10.14 | 0.4364 |
| ✗ | ✓ | 61.72 | 48.1 | 9.82 | 0.3393 |
| ✗ | ✗ | 58.65 | 35.4 | 9.75 | 0.3078 |
| **GPT-4 Evaluation** | | | | | |
| *Graph* | *Plan* | *NAT* | *COH* | *HELP* | *ACC* |
| ✓ | ✓ | 3.72 | 3.91 | 4.71 | 4.92 |
| ✓ | ✗ | 3.00 | 3.72 | 4.51 | 4.84 |
| ✗ | ✓ | 3.51 | 3.88 | 4.39 | 4.87 |
| ✗ | ✗ | 2.93 | 3.66 | 4.18 | 4.90 |

Coherence and Diversity Evaluation

| | | | Overall | | |
|---|---|---|---|---|---|
| **Baselines** | | | *Non-Live* | *Live* | *Overall* |
| **Claude-3.5-Sonnet** | | | **91.22** | 80.75 | 85.98 |
| **GPT-4-turbo-0409** | | | 90.28 | **85.02** | **87.65** |
| **GPT-4o-0513** | | | 85.02 | 78.20 | 81.61 |
| **LLaMA-3.1 8B** | | | 83.40 | 72.88 | 78.14 |
| | **Graph** | **Plan** | | | |
| **Ours** | ✓ | ✓ | 90.30 | 74.83 | 82.57 |
| | ✓ | ✗ | 89.60 | 73.71 | 81.66 |
| | ✗ | ✓ | 89.50 | 73.78 | 81.64 |
| | ✗ | ✗ | 89.00 | 73.18 | 81.09 |

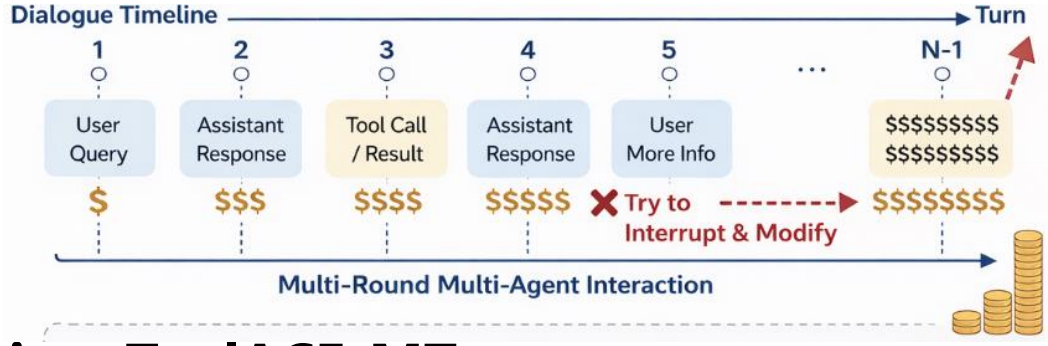
BFCL-v2 Performance



Zezhong Wang, Xingshan Zeng#, et al. "ToolFlow: Boosting LLM Tool-Calling Through Natural and Coherent Dialogue Synthesis." *NAACL 2025.*

# ToolACE-MT: Efficient and Controllable Generation

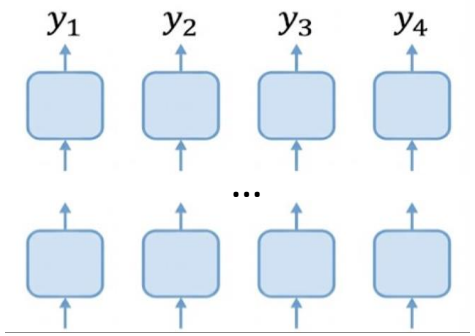
- **Limitation: Multi-Agent Simulation is costly and uncontrollable!**



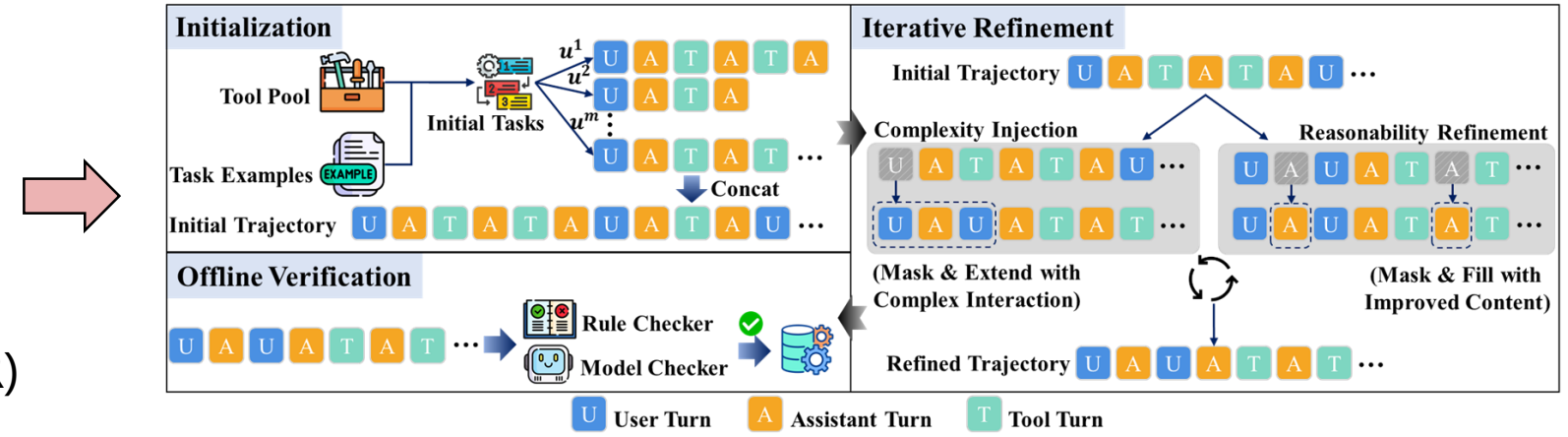

**Uncontrollable!**

**Costly!**

- **Our Solution: ToolACE-MT**
  - **Non-Autoregressive Generation:** Mask & Extend/Fill for iterative refinement




Non-Autoregressive (NAR)

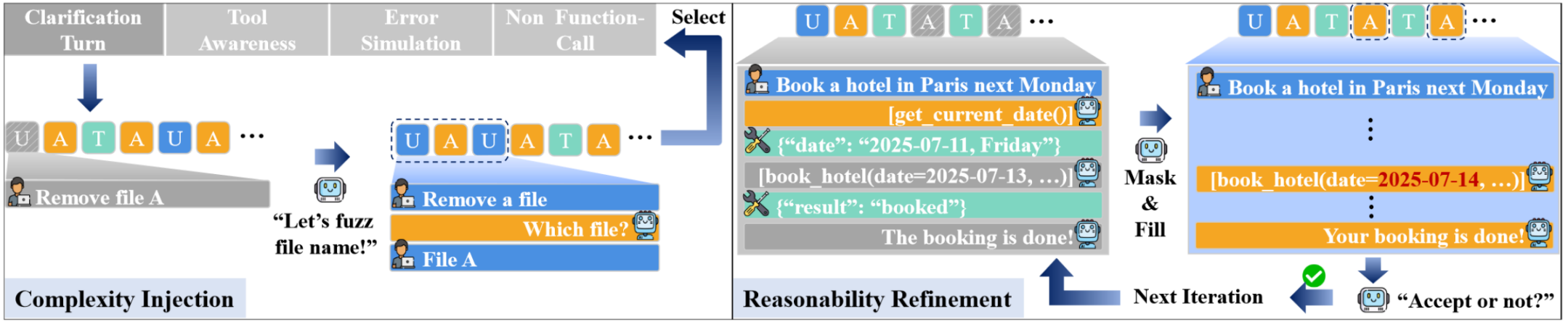





Xingshan Zeng, et al. "ToolACE-MT: Non-Autoregressive Generation for Agentic Multi-Turn Interaction." *ICLR 2026.*

# ToolACE-MT: Iterative Refinement

- **Complexity Injection**:
  - **Mask & Extend:** Clarification; Tool awareness; Error simulation; Non-FC; …
- **Reasonability Refinement**:
  - **Mask & Fill**: Mask and then recover the corresponding turns




Advantages

**More Efficient** when generating long-horizon dialogues!
**Controlled Generation:** The complexity can be controlled and injected.

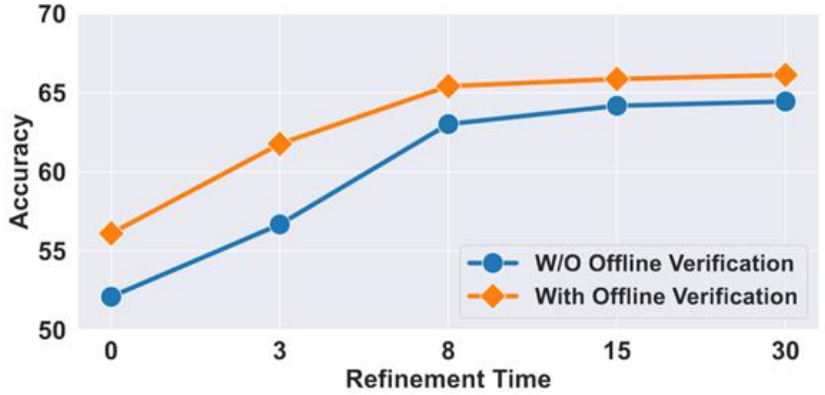


Xingshan Zeng, et al. "ToolACE-MT: Non-Autoregressive Generation for Agentic Multi-Turn Interaction." *ICLR 2026.*

# ToolACE-MT: Improved Efficiency

- Compared to MAS:
  - Much **less API calls**; Better quality.

- Refinement improves data quality:
  - Complementary to Offline Verification




Effects of Iterative Refinement

| Method | Cost | | | | Quality Performance | |
|---|---|---|---|---|---|---|
| | API Call times | Input (#) | Output (#) | Pricing (USD) | | |
| **MAS** with GPT-4o | 275k | 652,145k | 10,712k | 1,737 | 61.1 | 64.17 |
| **ToolACE-MT** with GPT-4o | 188k | 478,115k | 18,480k | 1,380 | 72.3 | 65.41 |
| **ToolACE-MT** with GPT-4o-mini | 394k | 855,391k | 33,062k | 148 | 48.7 | 60.13 |

Cost Comparison



Xingshan Zeng, et al. "ToolACE-MT: Non-Autoregressive Generation for Agentic Multi-Turn Interaction." *ICLR 2026.*

# Outline

- Overview of LLM-based Agents
- Scaling Capability: Scalable Agentic Data Generation
- **Improving Potential: Model-Aware Training and Inference Scaling**
- Summary and Future Horizons: Towards Next-Generation Agents

# From Better Data to Better Training

- Typical training:
  - **One-time** data selection
  - Direct training with a **fixed** dataset

- Two key observations:
  - Data suitability may be **model-dependent**
  - Model capability **changes during training**

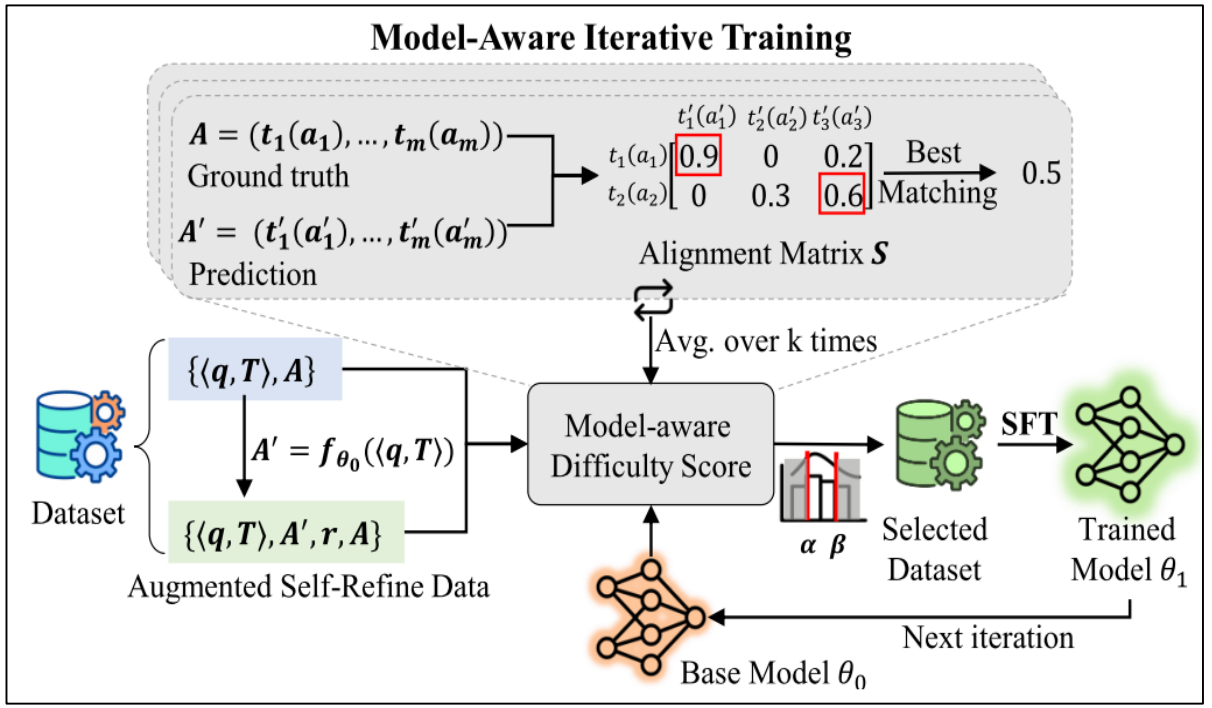



**Training data should adapt to both the model and its learning stage!**

# ToolACE-R: Model-Aware Iterative Training

- Target:
  - Improving the **data utilization** with limited training samples

- Our Solution:
- **Model-Aware Selection**:
  - Difficulty Score calculated with the model to be trained
- **Data Augmentation**:
  - Self-Refine Data: (q, A', r, A)
- **Iterative Training**:
  - Re-evaluate and select in each iteration

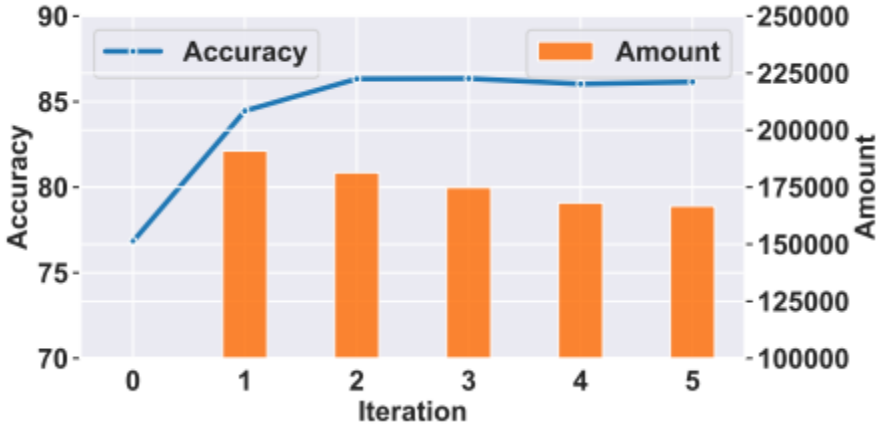





Xingshan Zeng, et al. "ToolACE-R: Model-aware Iterative Training and Adaptive Refinement for Tool Learning." *AAAI 2026.*

# ToolACE-R: Effects of Model-Aware Training

- Data Selection needs to be:
  - Model-aware
  - Within suitable scale
  - Better evaluated with more inference




Effect of Iterative Training

| Thresholds | Non-live | Live | Overall |
|---|---|---|---|
| $\alpha = 0, \beta = 0.9$ **(ToolACE-R)** | 90.94 | 81.72 | 86.33 |
| $\alpha = -1, \beta = 0.9$ | 90.73 | 81.27 | 86.00 |
| $\alpha = 0.1, \beta = 2$ | 89.27 | 81.35 | 85.31 |
| $\alpha = 0.1, \beta = 0.8$ | 90.83 | 80.38 | 85.61 |

Threshold Selection

| Models | Non-live | Live | Overall |
|---|---|---|---|
| $k = 8$ **(ToolACE-R)** | 90.94 | 81.72 | 86.33 |
| **+ Adaptive SR** | 91.32 | 82.34 | 86.83 |
| $k = 1$ | 90.94 | 80.98 | 85.96 |
| **+ Adaptive SR** | 90.71 | 82.01 | 86.36 |

Difficulty Eval with Small k

| Models | Live | Overall | Amount |
|---|---|---|---|
| **ToolACE-R** | 81.72 | 86.33 | 120K |
| **Select w/ Qwen2.5-3B** | 80.83 | 85.50 | 125K |
| **Select w/ Qwen2.5-7B** | 81.27 | 85.97 | 134K |
| **Intersection Data** | 81.37 | 86.08 | 108K |

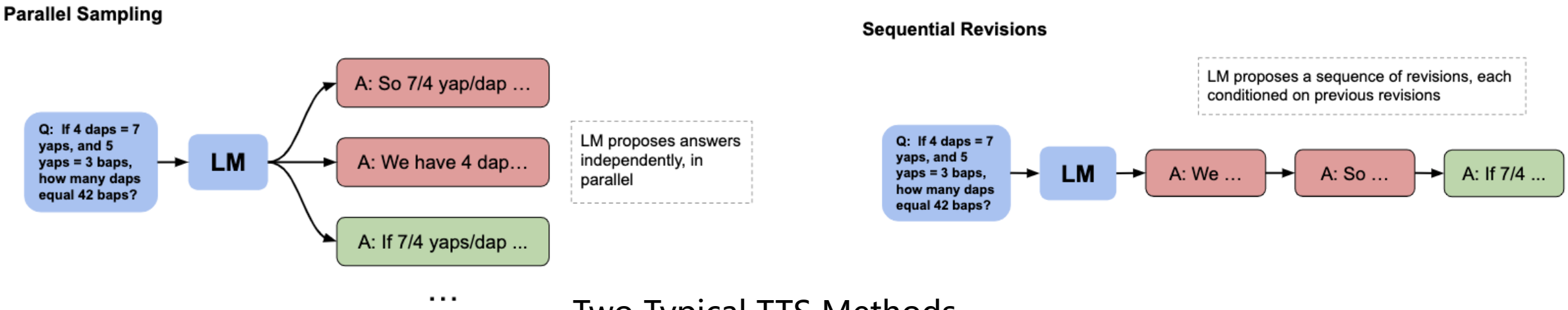
Difficulty Eval with Diff Models



Xingshan Zeng, et al. "ToolACE-R: Model-aware Iterative Training and Adaptive Refinement for Tool Learning." *AAAI 2026.*

# Towards Better Inference

- **Test-Time Scaling (TTS):**
  - **Improving performance by allocating more inference time**




Two Typical TTS Methods

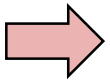
**Key Idea: Explore before Giving Final Answer**

# ToolACE-R: Adaptive Self-Refinement

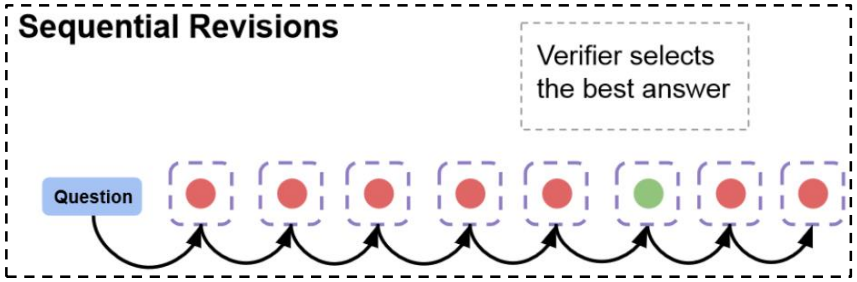
- **Challenge:** LLMs cannot realize correct answers during self-refinement.
- **Our Solution:**
  - **During training:** Data augmentation (q, A', r, A)

A'≠ A: Learn to refine incorrect invocation

A'= A: Learn to keep correct invocation

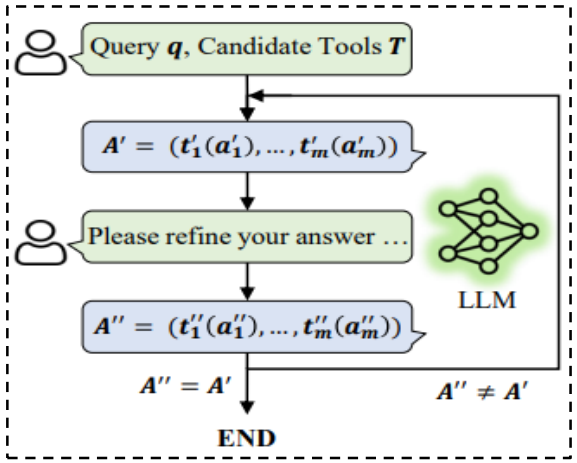


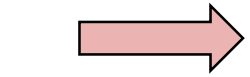
Learn to **Adaptive** Self-Refine!



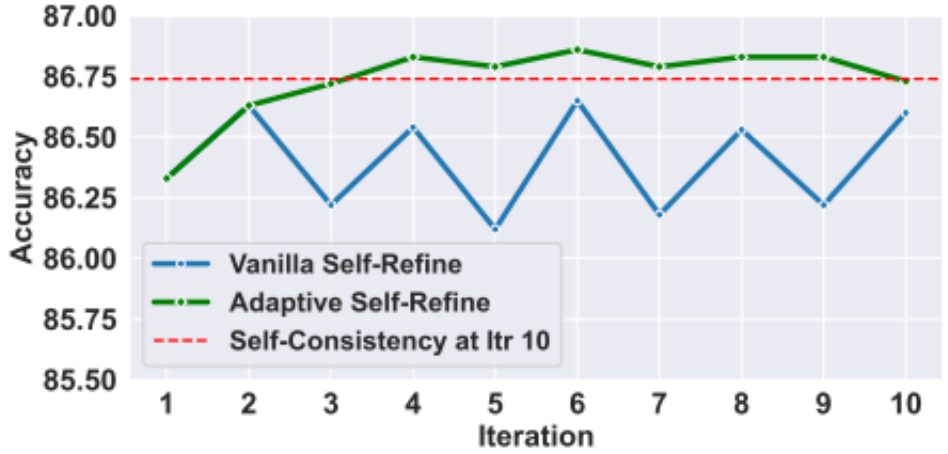

**Verifier is needed for selection!**

  - **During inference:** Adaptive Self-Refine



**No fluctuation!**






Xingshan Zeng, et al. "ToolACE-R: Model-aware Iterative Training and Adaptive Refinement for Tool Learning." *AAAI 2026.*

# ARTIS: Toward Agent-Centric Scaling

- **Agentic** vs. **Non-Agentic** Scenarios: **Environment!**
- **Challenge:** How to leverage **environment feedback** but not actually **taking risky actions**?
- **Motivation:** Human can do **Mental Rehearsal** before Taking Real Actions.







**ARTIS: Simulate before Action!**

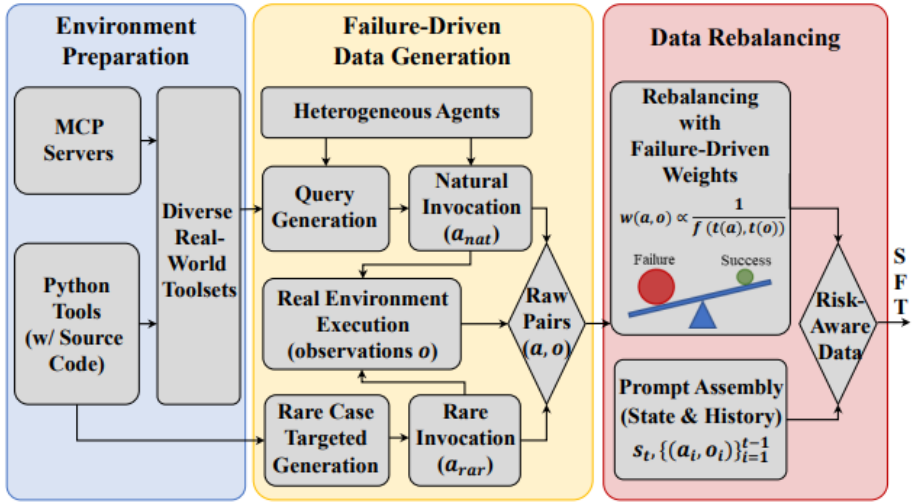
① Find the **best solution** path avoiding **costly** actions;
② Avoid problematic actions in **irreversible** scenarios!



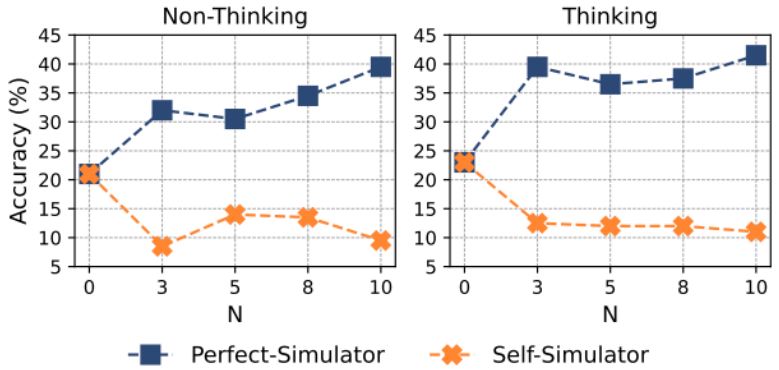
Xingshan Zeng, et al. "ARTIS: Agentic Risk-Aware Test-Time Scaling via Iterative Simulation." *2026.*

# ARTIS: Risk-Aware Simulator

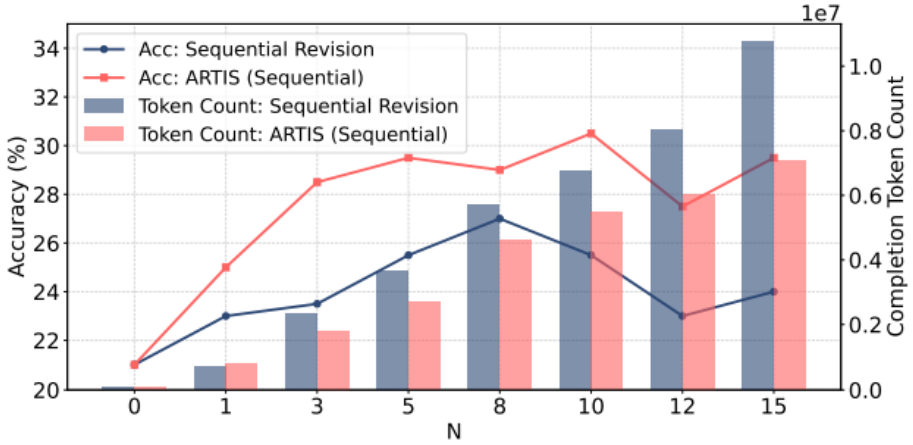
- Key Factor: **the Quality of Simulator!**
- **Risk-Aware Simulator Training:**
  - Failure-driven Generation
  - Data Rebalancing




Risk-Aware Simulator Training




Effects of Different Simulators




Compared to Sequential Revision



Xingshan Zeng, et al. "ARTIS: Agentic Risk-Aware Test-Time Scaling via Iterative Simulation." *2026.*

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- **Summary and Future Horizons: Towards Next-Generation Agents**

# Summary

## Complex Tool Use for Real-World Tasks

**Scalable, High-Quality Data Generation**

**Model-Aware Training**
(Better utilization of data)

**Agentic Test-Time Scaling**
(Better utilization of model)
(Reliability enhancement)

## A Holistic Data-Centric Paradigm

Next

## Beyond Complex Tool Use

- **Multi-Modal Tool Use**
- **Personalized Tool Use**
- **Proactive Tool Use**

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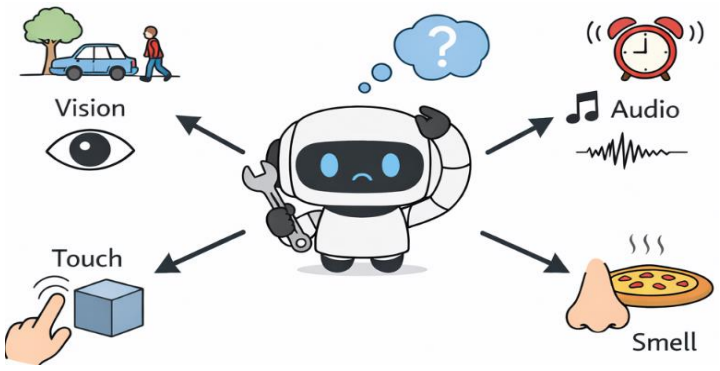
# Future Horizons

- **Universal Capability: Beyond Text-Only Tool Use**

**Real-world tasks are inherently multi-modal and require broader interactions!**

- **Multi-Modal Tool Use**
  - Multi-modal perception
  - Orchestrating multi-modal tools
  - …

- **Toward Universal Multi-Modal Agents**
  - Unified representation across modalities
  - Cross-modal reasoning and planning
  - …



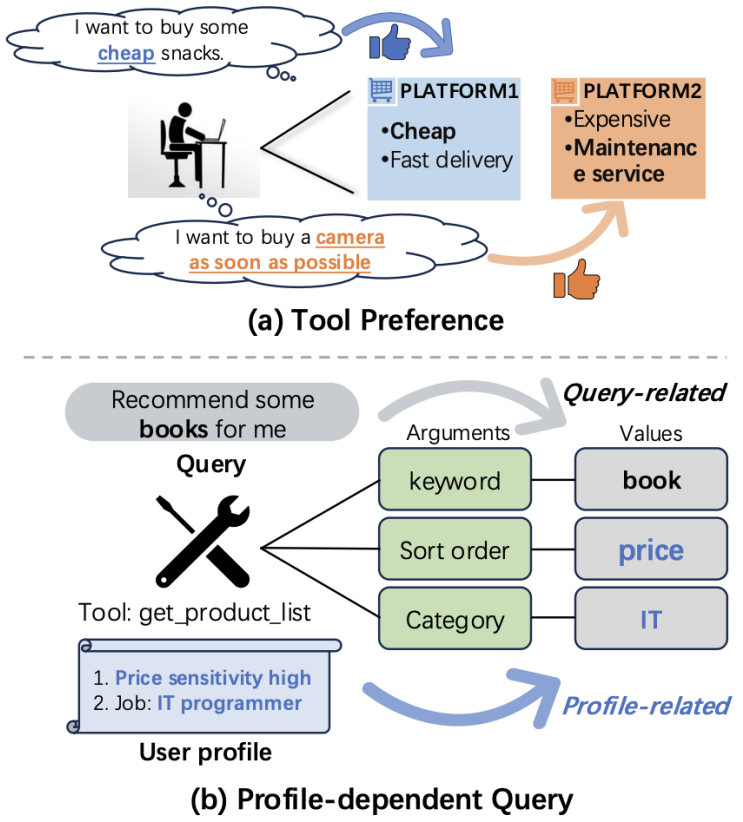
# Future Horizons

- **Adaptive Intelligence: Personalized Tool Use**

**Real-world tasks should be user-specific!**

- **Tool Preference**
  - Users might exhibit specific preferences over tools with similar functionalities.
  - E.g., online shopping tools: JD vs TB?

- **Profile-dependent Query**
  - Users tend to express their needs concisely and omit crucial details, which can be inferred from user profile.
  - E.g., travel planning: A likes shopping, B like natural scenery.






Xu Huang, et al. " Advancing and Benchmarking Personalized Tool Invocation for LLMs" *2025.*

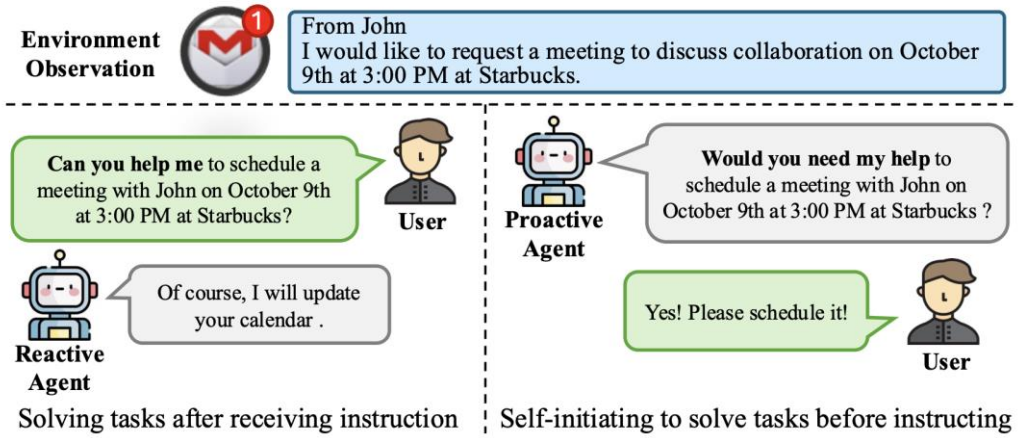
# Future Horizons

- **Proactive Tool Use: Self-Evolution**

**Real-world Environments are Dynamic!**

- **From Reactive to Proactive Tool Use**
  - Reactive Tool Use: Actions are only taken when receiving tasks
  - Proactive Tool Use: Take actions based on the environment states

- **Self-Evolution**: Adaptive to the environment
  - Continual/Online learning
  - Experience/Skills generation
  - …









Yaxi Lu, et al. "Proactive agent: Shifting llm agents from reactive responses to active assistance" *ICLR 2025.*

# Towards Next-Generation Autonomous Agents

**Complex Tool Use for Real-World Tasks**



**Scalable, High-Quality Data Generation**



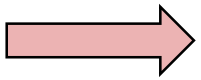
**Model-Aware Training**
(Better utilization of data)



**Agentic Test-Time Scaling**
(Better utilization of model)
(Reliability enhancement)

**A Holistic Data-Centric Paradigm**

Next



**Beyond Complex Tool Use**

- **Multi-Modal Tool Use**
- **Personalized Tool Use**
- **Proactive Tool Use**

**More Directions**

- **Broader capabilities**
  - **Planning/Memory/…**
- **Enhanced adaptivity**
  - **Domain/Device/Fast Apply/…**

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# Thank you!