香港科技大學
THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY

COMP 4901B

Large Language Models

Language Agents and Tools

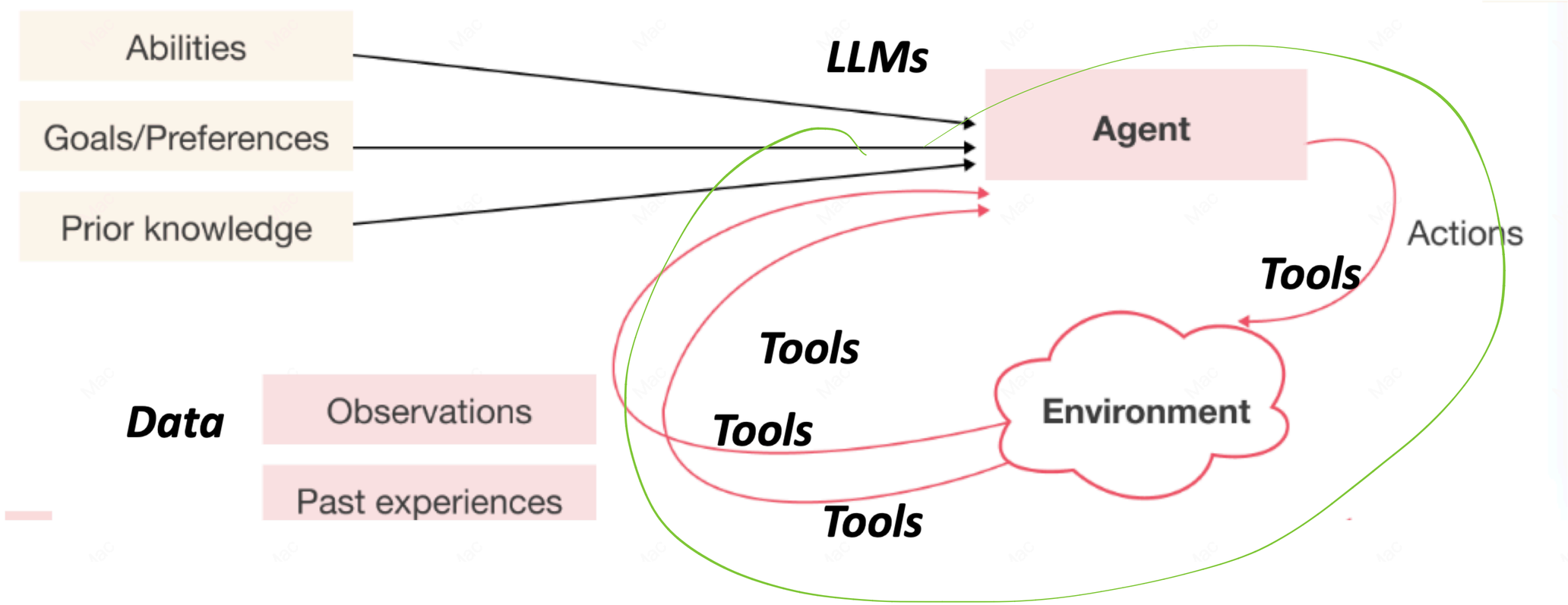
Junxian He

Nov 12, 2025

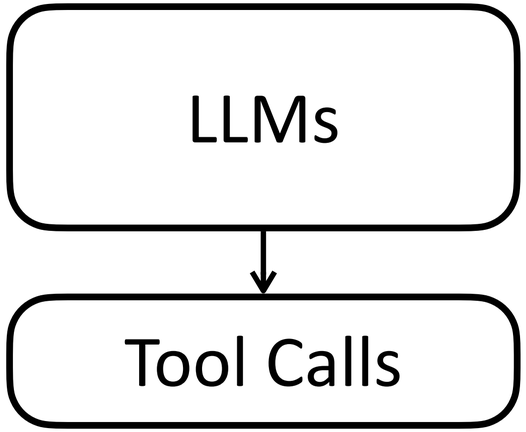
Part of slides are adapted from CMU 11711

Recap: What are Agents

Anything that can be viewed as **perceiving** its environment through sensors and **acting** upon that environment through actuators.



One-Step Tool Call -> Agents



not exact

```
{
  "response": "Sure, I'll check the current weather for you.",
  "reasoning": "I need real-time conditions so the user's route recommendation is accurate.",
  "tool_calls": [
    {
      "name": "get_weather",
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      }
    }
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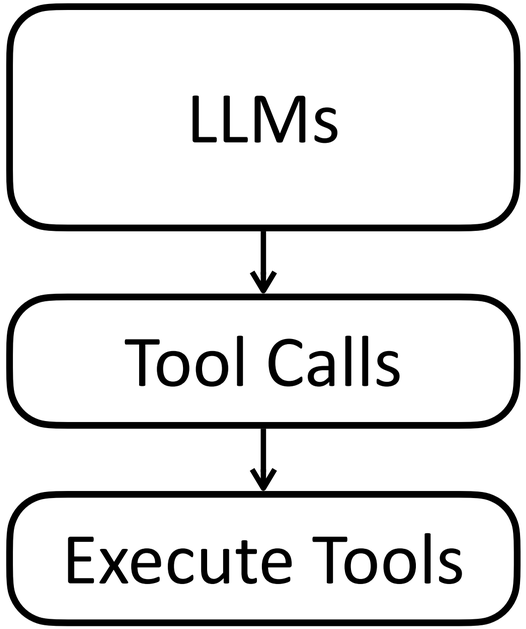

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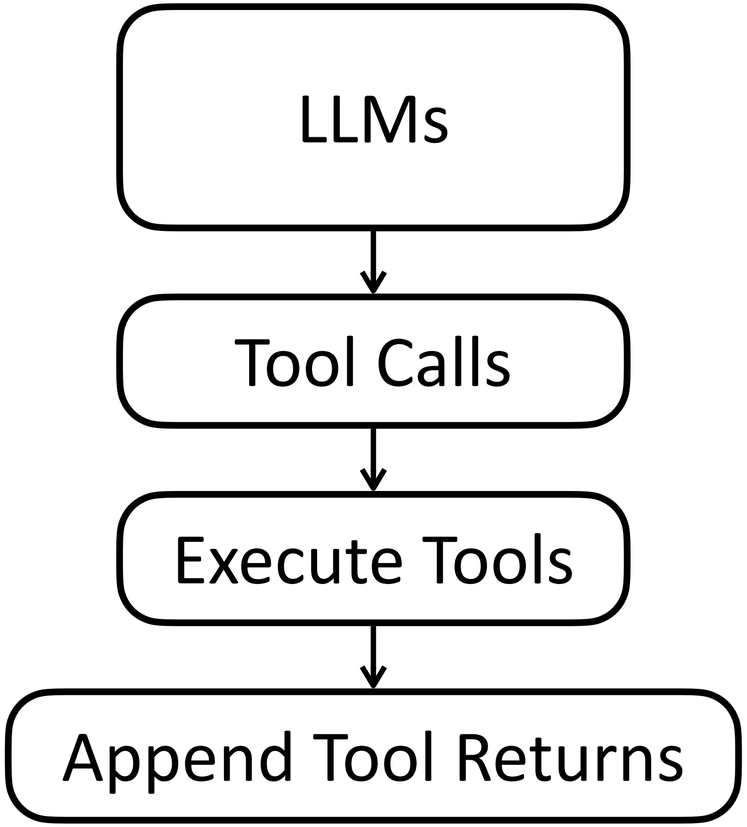


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    }
  ],
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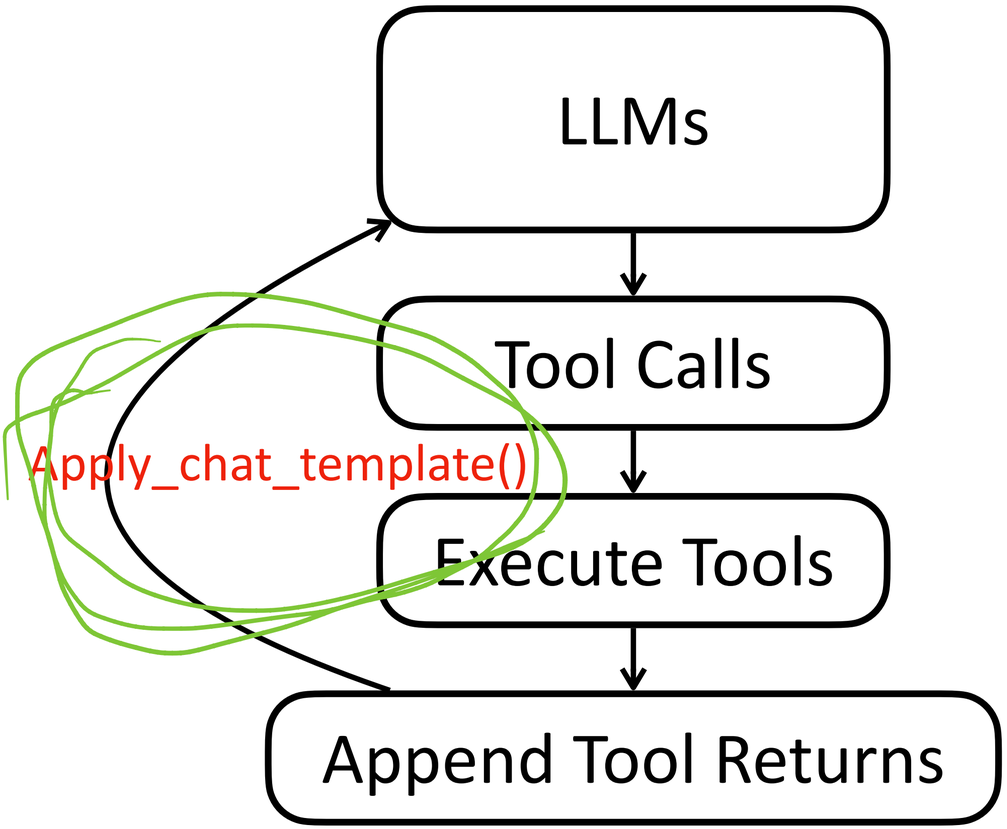


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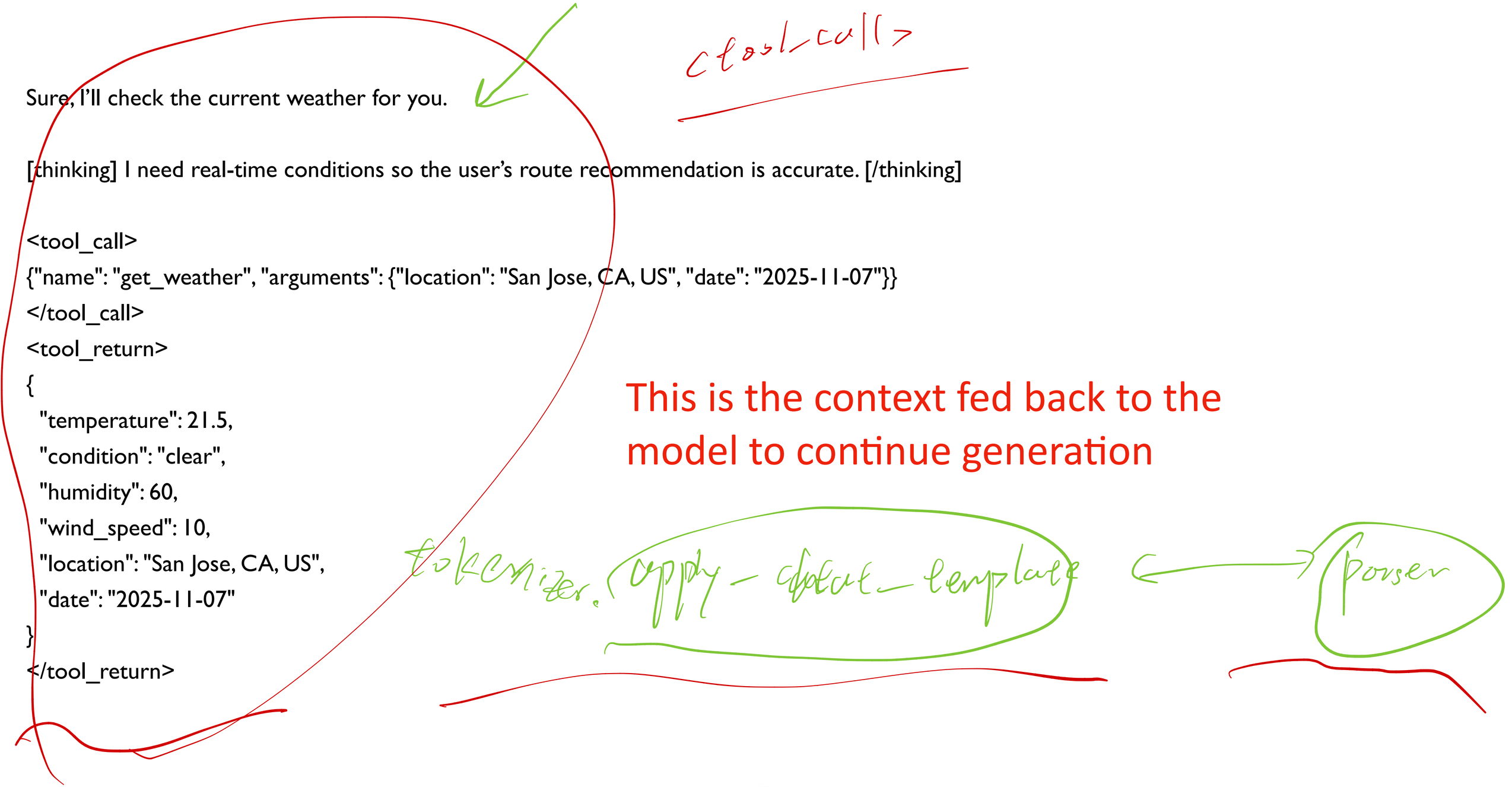

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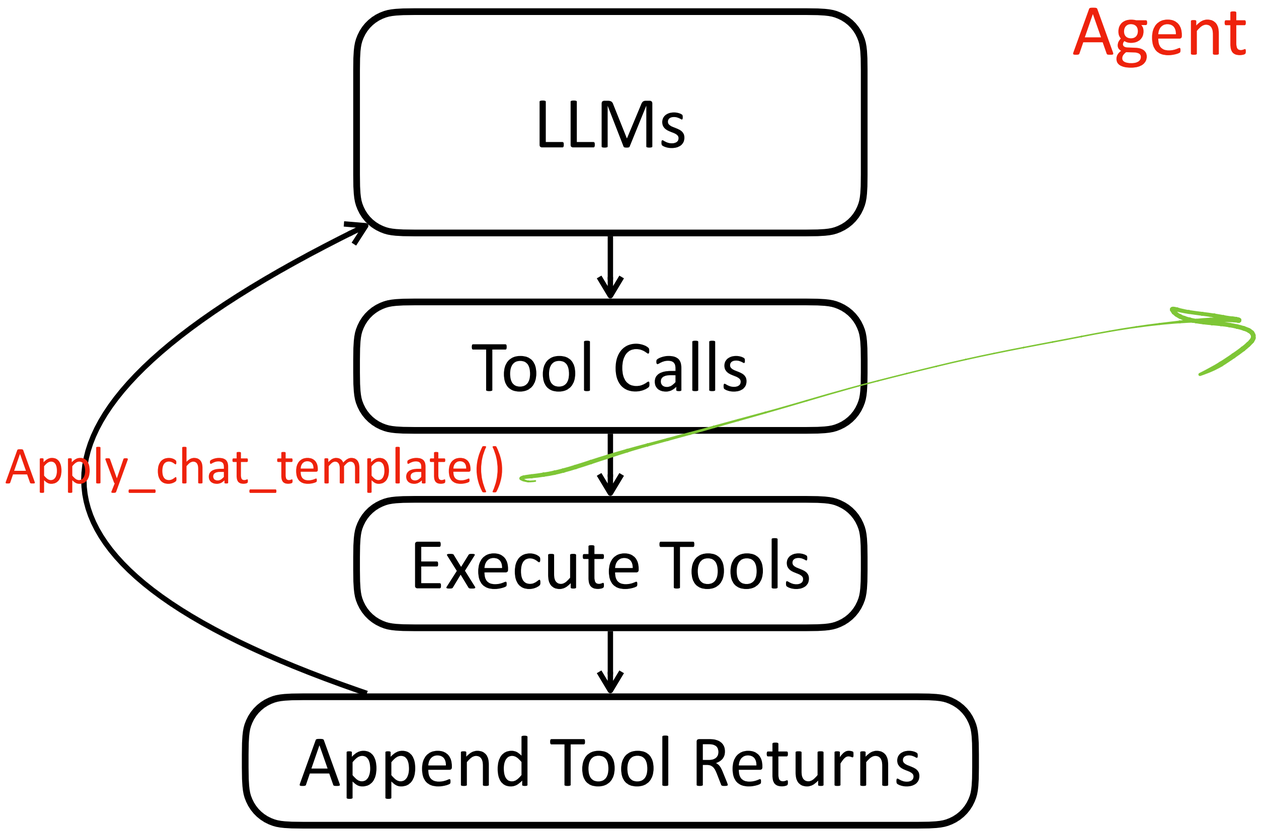

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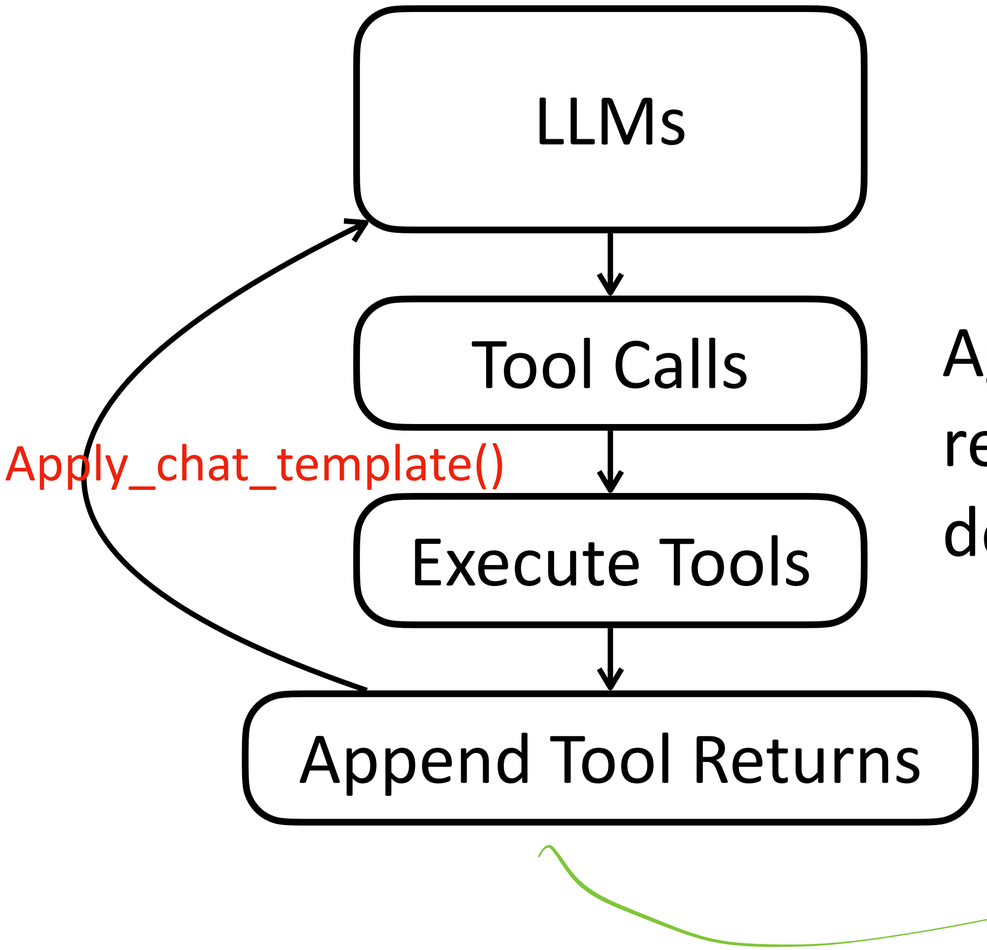


Agent Loop

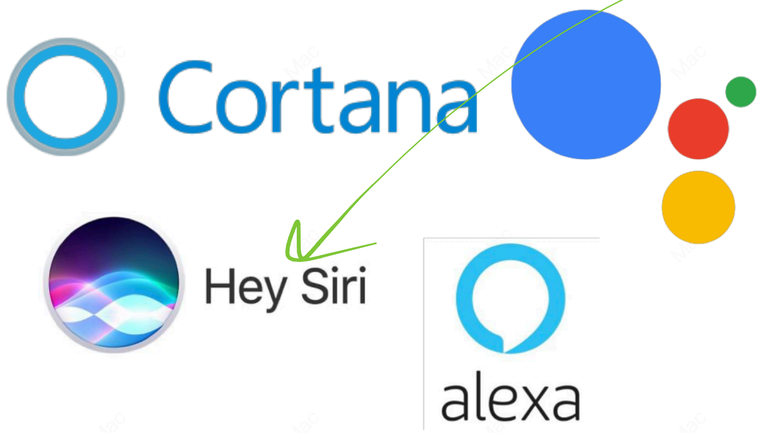
Agent loop ends when the model generates a text response without tool calling, or sometimes we define a “done” tool for the model to call

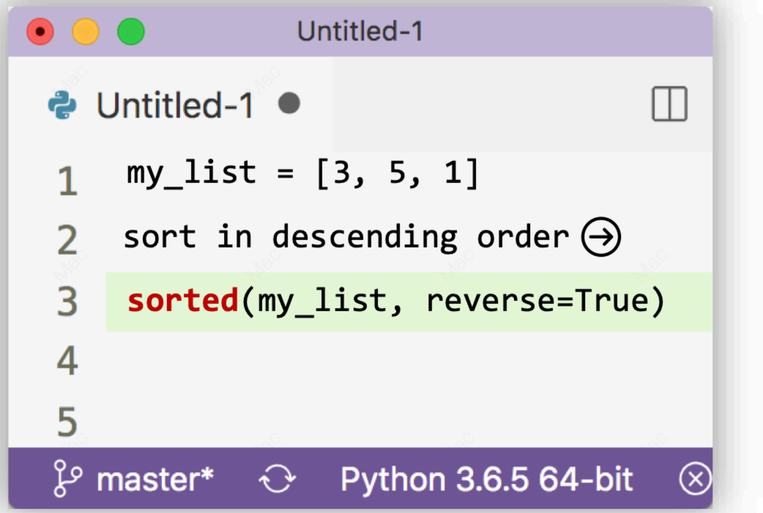
One-step Example

```python
def send_messages(messages):
    response = client.chat.completions.create(
        model="deepseek-chat",
        messages=messages,
        tools=tools
    )
    return response.choices[0].message

client = OpenAI(
    api_key="<your api key>",
    base_url="https://api.deepseek.com",
)

tools = [
    {
        "type": "function",
        "function": {
            "name": "get_weather",
            "description": "Get weather of a location, the user should supply a location first.",
            "parameters": {
                "type": "object",
                "properties": {
                    "location": {
                        "type": "string",
                        "description": "The city and state, e.g. San Francisco, CA",
                    }
                },
                "required": ["location"]
            },
        }
    },
]

messages = [{"role": "user", "content": "How's the weather in Hangzhou, Zhejiang?"}]
message = send_messages(messages)
print(f"User>\t {messages[0]['content']}")

tool = message.tool_calls[0]
messages.append(message)

messages.append({"role": "tool", "tool_call_id": tool.id, "content": "24℃"})
message = send_messages(messages)
print(f"Model>\t {message.content}")
```

Why Do We Want Agents

Imagine if things get done by just talking…





Virtual Assistants

- *Set an alarm at 7 AM*
- *Remind me for the meeting at 5pm*
- *Play Jay Chou's latest album*

Natural Language Programming

- *Sort my_list in descending order*
- *Copy my_file to home folder*
- *Dump my_dict as a csv file output.csv*

Training-free Methods for Building Agents

How to Let LLM Become an Agent

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Sure, I'll check the current weather for you.

[thinking] I need real-time conditions so the user's route recommendation is accurate. [/thinking]

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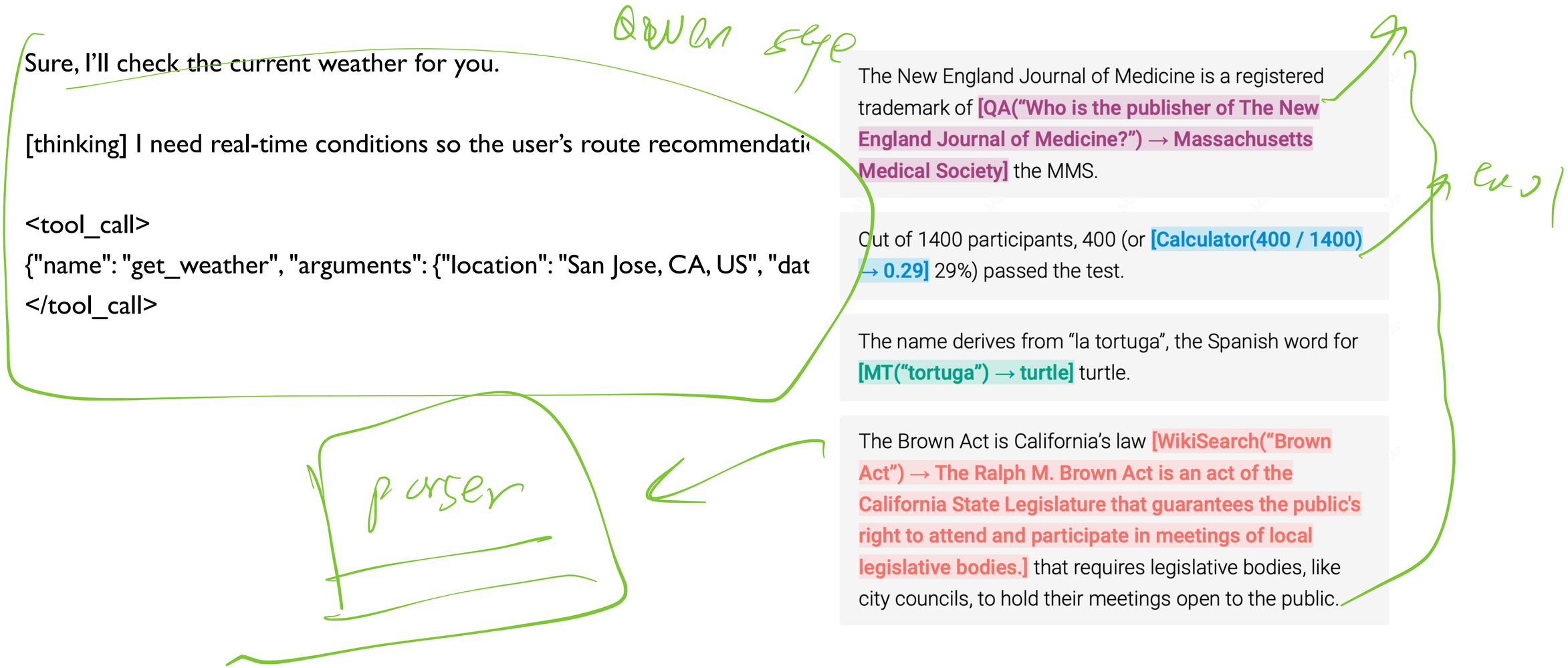

We just need the LLMs to output certain formats of tool calls that we can parse

Just Prompt

Supposing you have the following APIs, answer the given question.

Available APIs:
1. weather(location): for getting the weather information given a location
2. location(): for getting the location of the user.
3. bus_route(start, end): for finding the current bus route from the start position to the end position.
4. count_characters(s): for counting the number of characters in a string s.

Question: Is it okay to go hiking today?

To know the answer, we first need to know the current location of the user.
API call: location() = Seattle.
Next, we need to know the current weather in Seattle.
API call: weather(Seattle) = Cloudy with a chance of rain.

Based on this information, it is not recommended to go hiking today in Seattle.

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Question: how long does it take to take a bus to Vancouver?

To answer this question, we first need to know the current location of the user.
API call: location() = Seattle.
Next, we need to find the bus route from Seattle to Vancouver.
API call: bus_route(Seattle, Vancouver) = 4 hours.

Therefore, it takes 4 hours to take a bus from Seattle to Vancouver.

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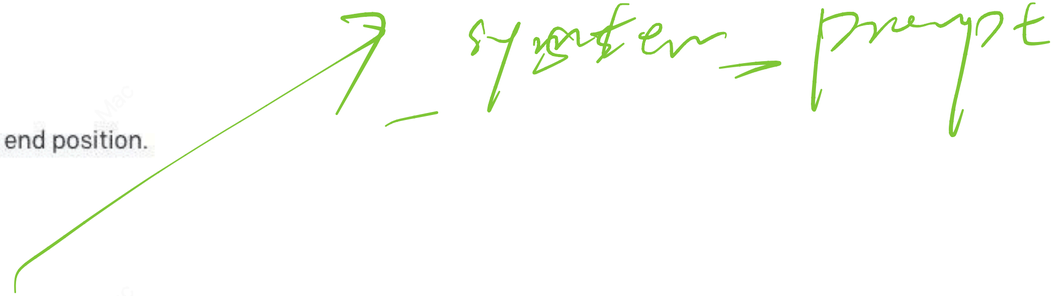

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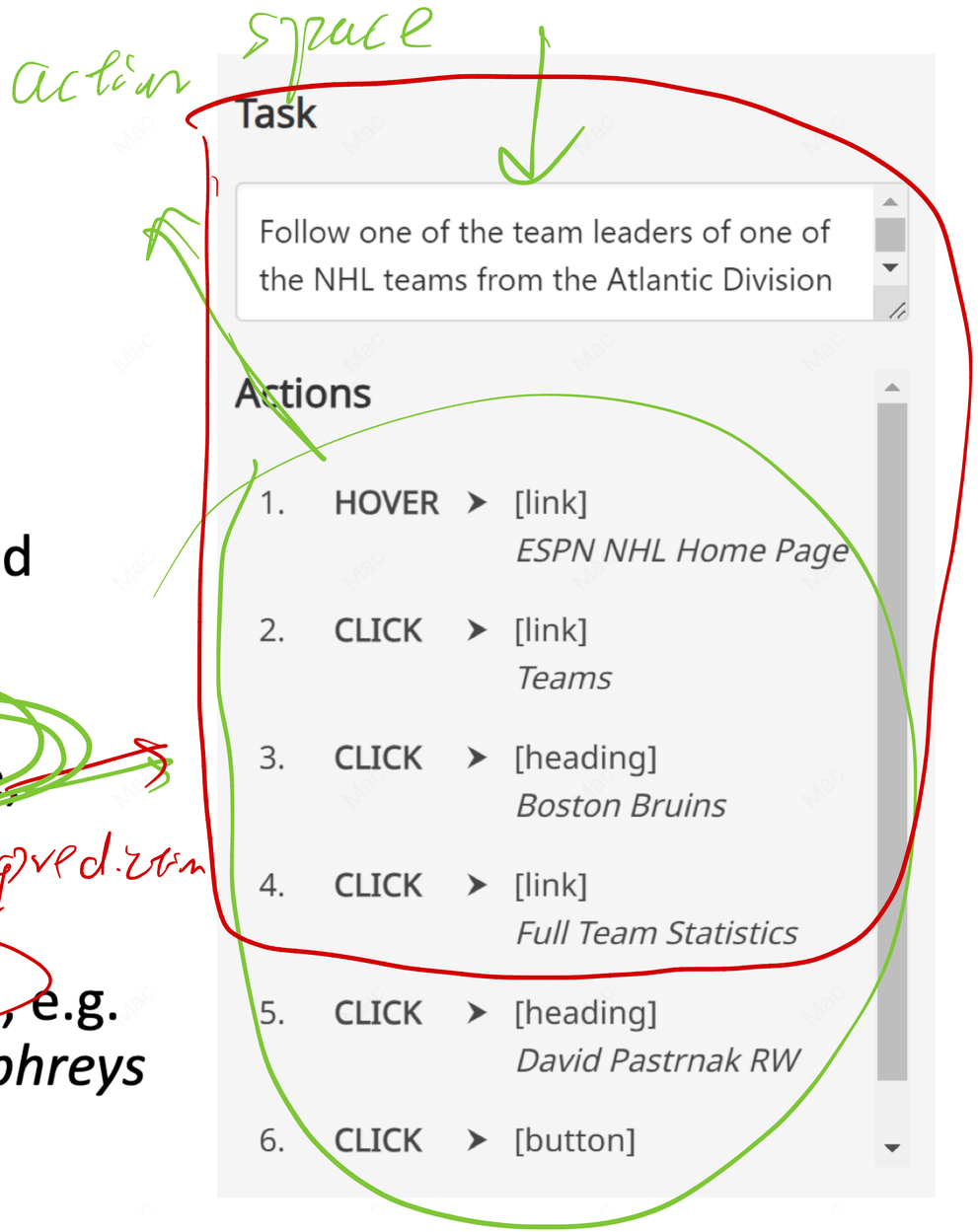
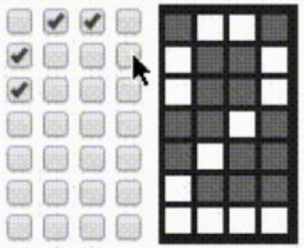
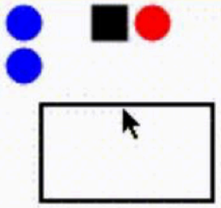
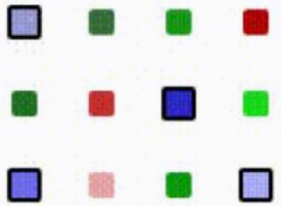
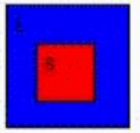
Evaluating Language Agents

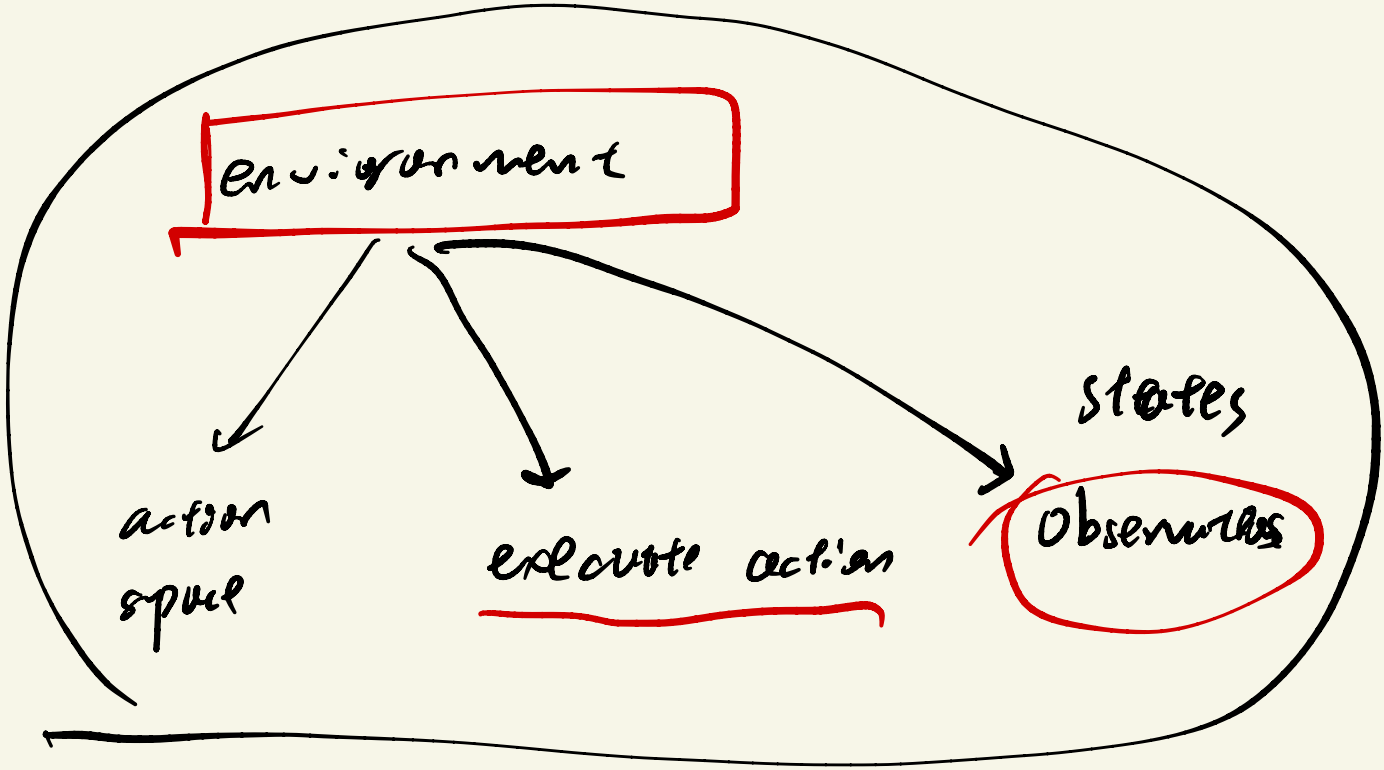
Evaluation of LLM Agents

- Simplified environments and basic tasks
- Performance is saturating.

1. Stateless, non interactive environment, e.g. *Mind2Web (Deng et al. 2023)* has only dumped pages.
2. Checking action sequence accuracy (step-wise, surface form only)
3. Simple interactive environment, short horizon, e.g. *WebShop (Yao et al. 2023), MiniWoB++ (Humphreys et al. 2022)*



Move the cube around so that "**5**" is the active side facing the user.	Set the sliders to the combination [13,20,13] and submit.	Draw the number "2" in the checkboxes using the example on the right and press Submit when finished.	Drag Ree to the 4th position.	Keep your mouse inside the circle as it moves around.	Enter the value of **Country** into the text field and press Submit.
 Submit	14 19 17 Submit	 Submit	Jade Ree Karlen Millie Noelyn		Gender: Male; First name: Annecorinne; Country: Guam; Year of Birth: 1934; Religion: Hinduism Submit
Drag all triangles into the black box.	Select 09/23/2016 as the date and hit submit.	Sort the numbers in increasing order, starting with the lowest number at the top of the list.	Copy the text from the **1st** text area below and paste it into the text input.	Select all the shades of blue and press Submit.	Find the **4th word** in the paragraph, type that into the textbox and press "Submit".
 Submit	Date: Sub September 2016	9 -12 49 -28 Submit	Blandit quisque. Amet ac odio aliquam. Ultrices ornare Submit	 Submit	Non arcu ut ultricies est. Gravida gravida. Porta erat nulla eget condimentum posuere a Submit
Click the button in the dialog box labeled "Cancel".	Highlight the text in the paragraph below and click submit.	Highlight the text in the paragraph below and click submit.	Find the **11th word** in the paragraph, type that into the textbox and press "Submit".	Move the cube around so that "**2**" is the active side facing the user.	Drag the smaller box so that it is completely inside the larger box.
Massa. Facilisi luctus. Est vel. Cancel OK	Submit Ultricies. Sagittis in.	Tempor posuere nibh. Vel nisl, faucibus. Feugiat condimentum Submit	Ullamcorper aliquet amet ullamcorper. Elit. Mattis luctus diam. Lobortis nulla fermentum ornare faucibus Submit	 Submit	 Submit


environment
action space
execute action
states
Observations

Instruction: i am looking for x-large, red color women faux fur lined winter warm jacket coat, and price lower than 70.00 dollars

Current Query: women fur jacket coat

Results

Page 1 (1-10) of 50 total results

Back to Search | Next >

B09KP78G37

Women Faux Fur Lined Jacket Coat Winter Warm Thick Fleece Outwear Trench Zipper Plus Size Long Sleeve Plush Overcoat

B07ZXBGDXF

Women's Coat, FORUU Winter Faux Fur Fleece Outwear Warm Lapel Biker Motor Aviator Jacket

B098XT346Y

Fjackets Real Lambskin Sherpa Jacket - Mens Leather Jacket

4.7

Current Action: `click[Fjackets Real Lambskin...]`

Key to Agent Benchmarks

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Environment:

- Diverse functionality.
- Rich and realistic content.
- Interactive
- Easily Extendable
- Reproducible

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Evaluation:

- Reliable metrics
- Encourage final goal rather than partial satisfaction.

WebArena

Environment:

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A sandbox Internet:

- Open source, production-ready implementation of the websites
- Data populated from real-world websites
- Easily distributable – Dockers, AWS images, etc.

simulate

WebArena (Zhou et al. 23')

Example Tasks in WebArena

sequence of actions

"Create a plan to visit Pittsburgh's art museums with minimal driving distance starting from Schenley Park. Log the order in my "awesome-northeast-us-travel" repository"

webarena.wikipedia.com

Wikipedia | Pittsburgh museums

List of museums in Pittsburgh

This **list of museums in Pittsburgh, Pennsylvania** encompasses museums defined for this context as institutions (including nonprofit organizations, government entities, and private businesses) that collect and care for objects of cultural, artistic, scientific, or historical interest and make their collections or related exhibits available for public viewing. Also included are university and non-profit art galleries. Museums that exist only in cyberspace (i.e., virtual museums) are not included.

Wikimedia Commons has media related to ***Museums in Pittsburgh***.

See also: List of museums in Pennsylvania

▾Museums

Search for museums in Pittsburgh

webarena.openstreetmap.com

OpenStreetMap | Edit | History | Export

Schenley Park, Pittsburgh, Allegheny County

The Andy Warhol Museum, 117, Sandusky Str

Car (OSRM) | Go

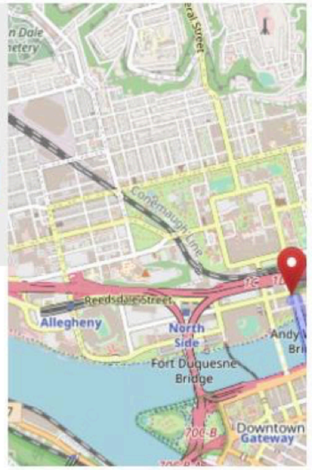
Reverse Directions

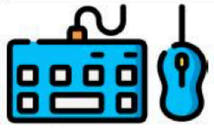
Directions

Distance: 7.1km. Time: 0:10.

1. Start on **Panther Hollow Road** 300m

2. Slight right onto unnamed road 160m





Search for each art museum on the Map

webarena.gitlab.com

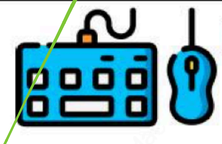
Update README.md

README.md 158 B | Edit | Replace

Travel in Northeast US

Pittsburgh

```
+ Miller Gallery at Carnegie Mellon University
+ American Jewish Museum
+ Carnegie Museum of Art
```



Record the optimized results to the repo

Outcome/Execution-based Evaluation

realistic

final

Goal: directly validate the correctness of the execution

- "When was the last time I bought shampoo?"
- **Directly compare with the annotated answer:** Answer is "Dec 15th, 2022"

More answers

Outcome/Execution-based Evaluation

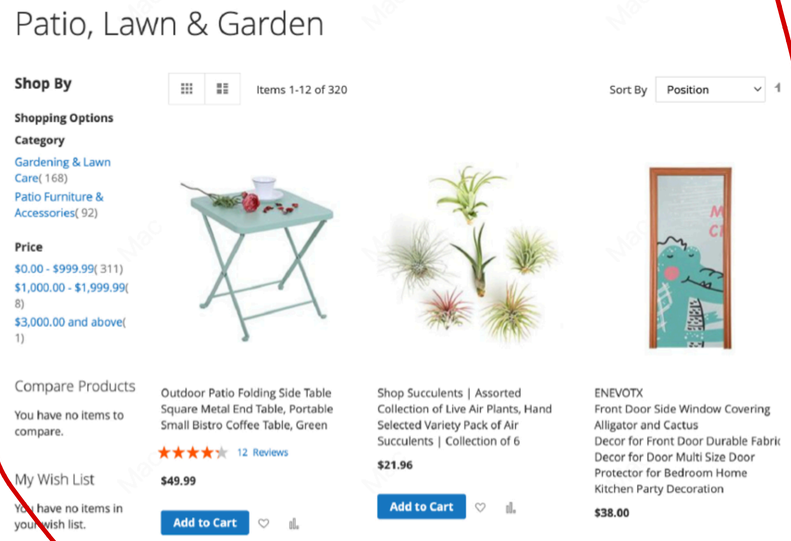
Post my question, "is car necessary in NYC", in a subreddit where I'm likely to get an answer

"f/nyc" in page.url

"Is car necessary in NYC?" in document.querySelector(".submission__inner").outText

Observation & Action Space

webarena.onestopshop.com



Screenshot

webarena.onestopshop.com

```
<li>
  <div>
    <a href="..."><img src="..."></a>
    <div class>
      <a href="...">Outdoor Patio …
</a>
      <div>
          <span>Rating:</span>
          <div>
            <span>82%</span>
          </div>
          <a href="…#reviews">12
<span>Reviews</span></a>
```

Text

webarena.onestopshop.com

```
RootWebArea 'Patio, Lawn ..'
  link 'Image'
    img 'Image'
  link 'Outdoor Patio..'
  LayoutTable ''
    StaticText 'Rating:'
    generic '82%'
    link '12 Reviews'
  StaticText '$49.99'
  button 'Add to Cart' focusable: True
  button 'Wish List' focusable: …
  button 'Compare' focusable: …
```

Accessibility tree

Keyboard: type

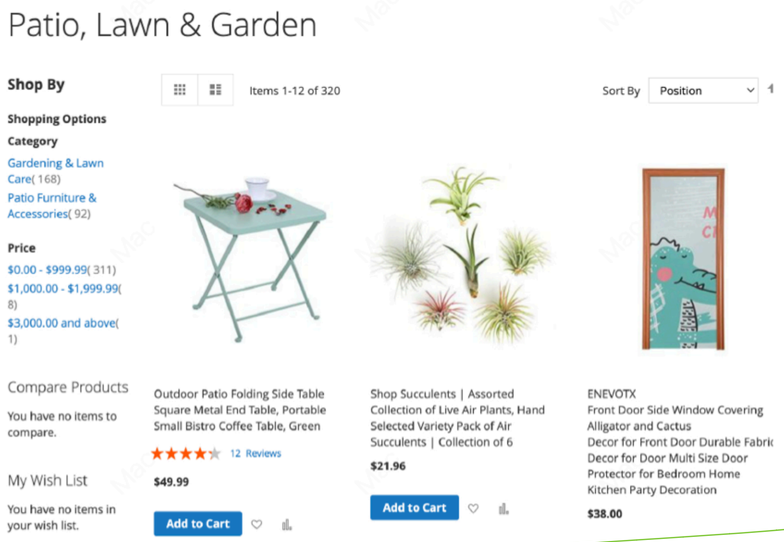
Mouse: click, hover, scroll

Browser: New tab, go back

flexible

Observation & Action Space

webarena.onestopshop.com



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Mouse: click, hover, scroll

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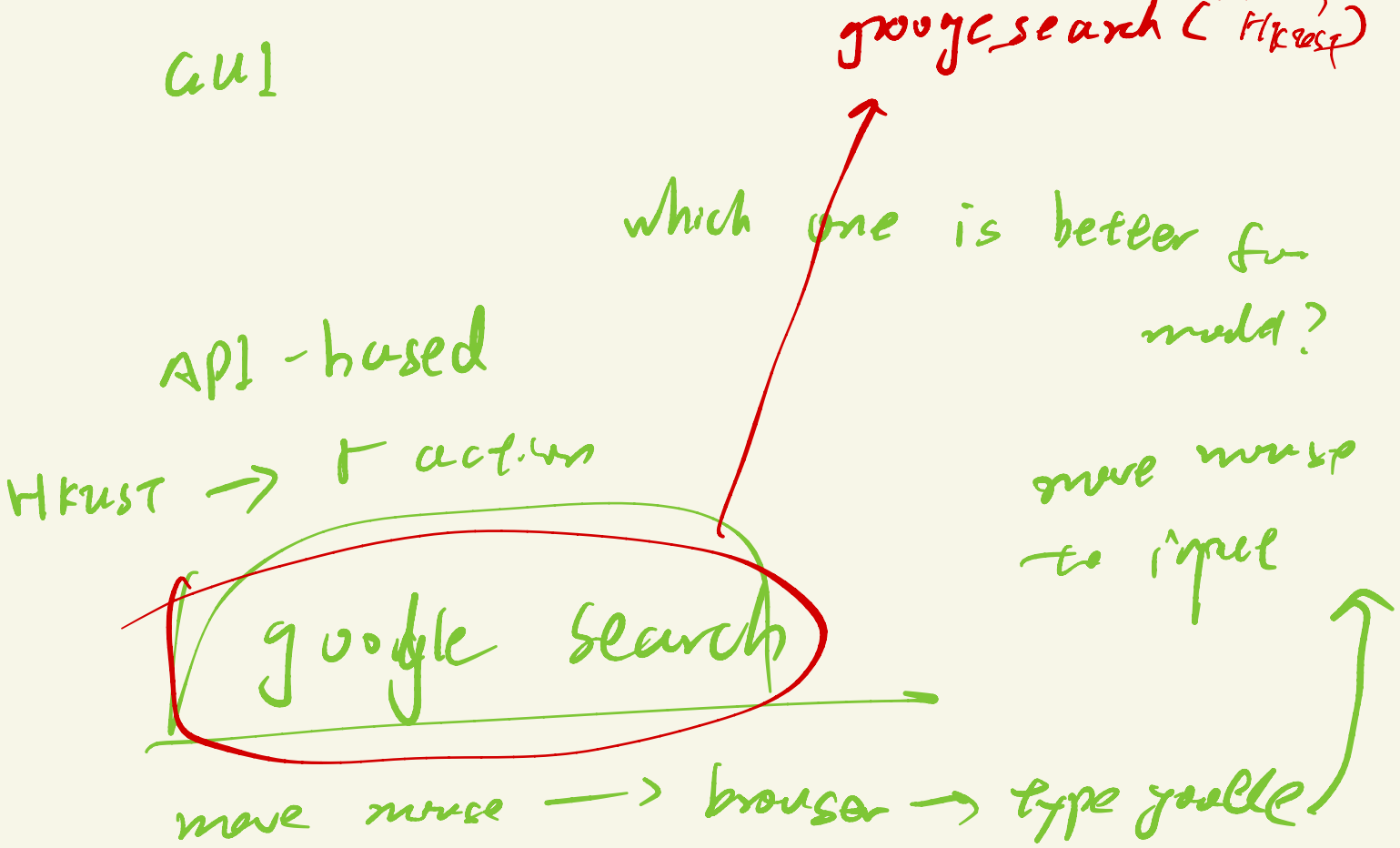
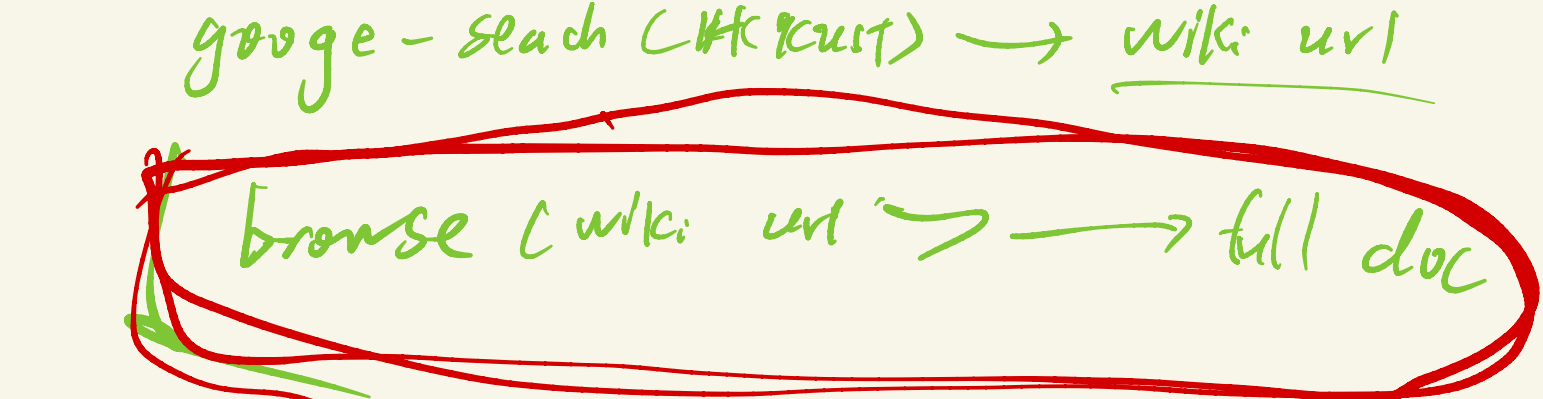
Another type of web agents, GUI agents, directly takes image as input observations


GUI
google_search('HKUST')
which one is better for model?
API-based
HKUST → function
move mouse to input
google search
move mouse → browser → type google

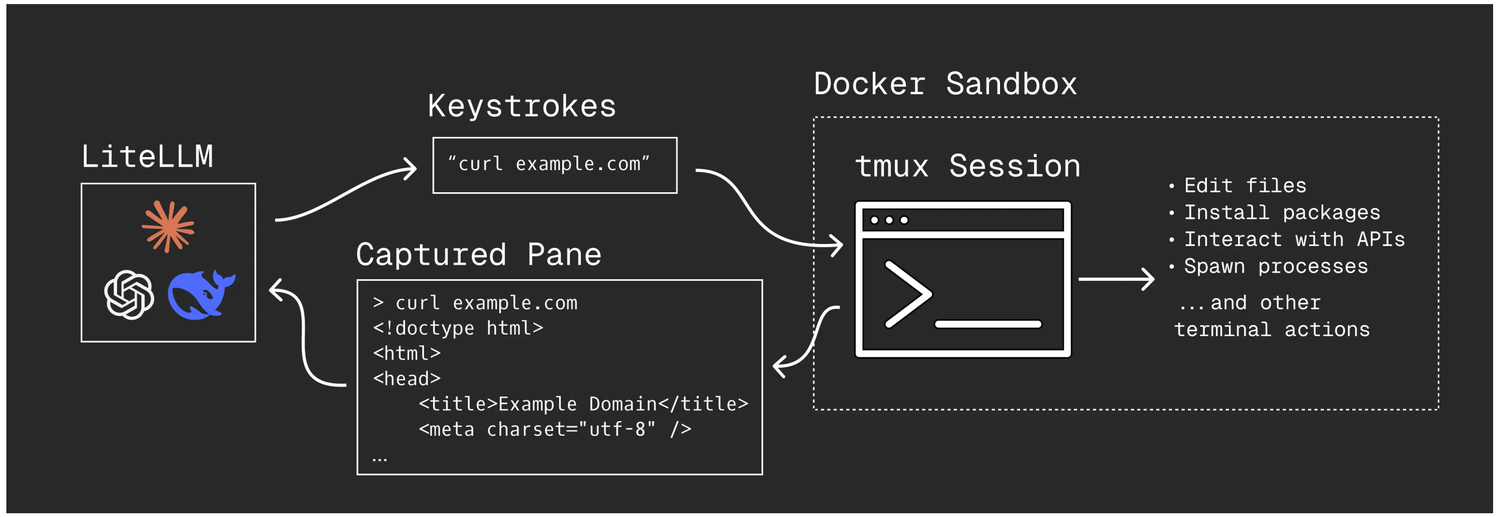
browse Wiki House page

screenshot → scroll down → screenshot

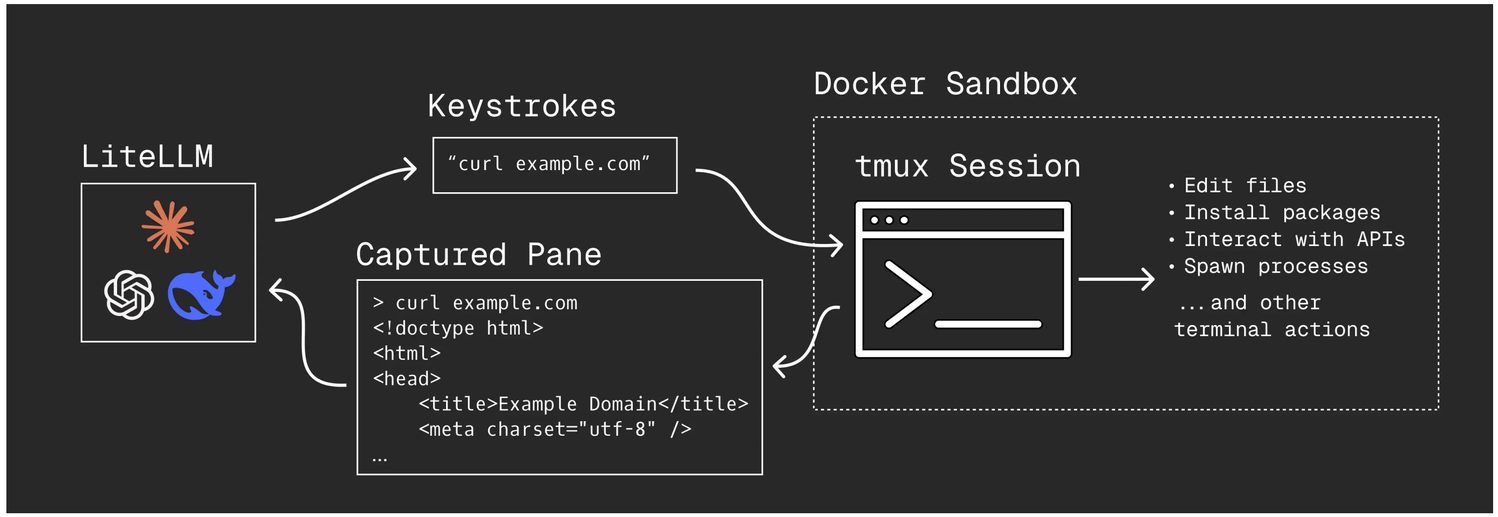
models:



TerminalBench



TerminalBench



Terminal-Bench: Possible Agent Actions

- Run shell commands (`ls` , `cd` , `make` , `python` , etc.)
- Manage tmux sessions/panes (`new-session` , `split-window` , `select-pane`)
- Edit files (`vim` , `nano` , `echo > file` , etc.)
- Install/build software (`apt install` , `gcc` , `make`)
- Read & analyze outputs/logs (`cat` , `less` , `grep`)
- Navigate directories and view help (`cd` , `ls` , `--help`)
- Verify or fix results (re-run scripts, check outputs)

Training Methods for Improving Agents

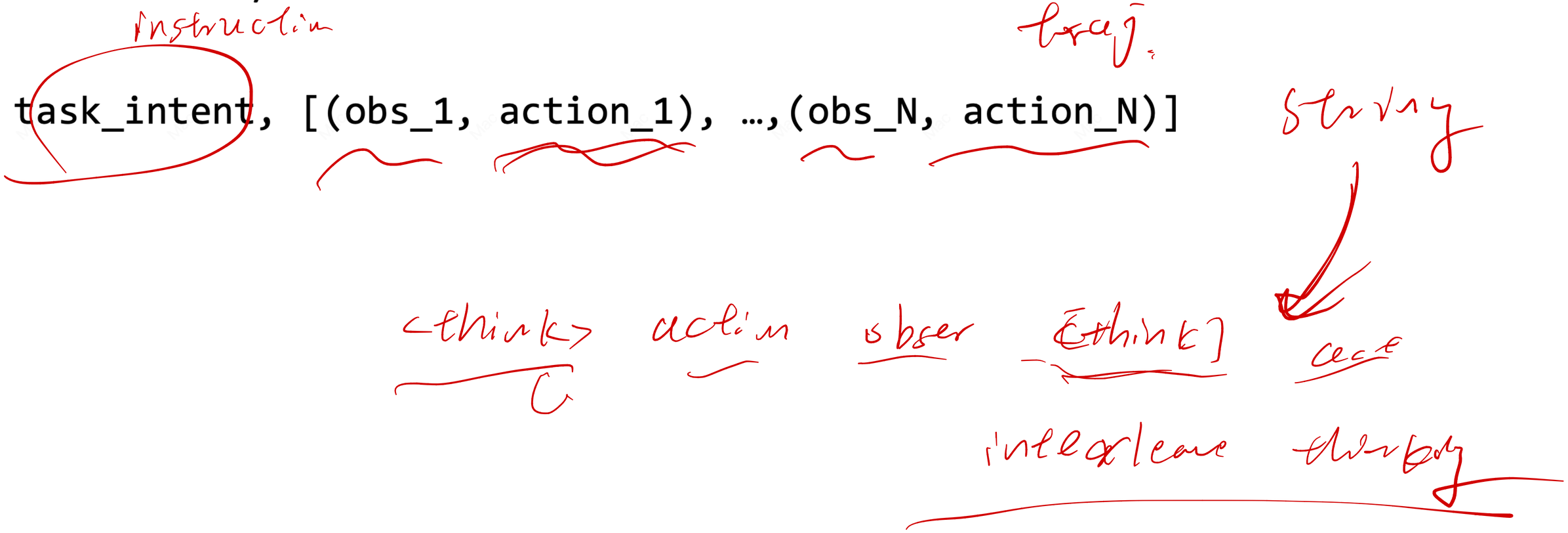
Learning of LLM Agents

- In-Context Learning – Learning from few-shot exemplars
- Supervised Finetuning – Learning From *Experts*
- Reinforcement Learning – Learning from *Environment*

Supervised Finetuning

- Collect large amount of expert trajectories (e.g. from human annotation)

```
task_intent, [(obs_1, action_1), …,(obs_N, action_N)]
```



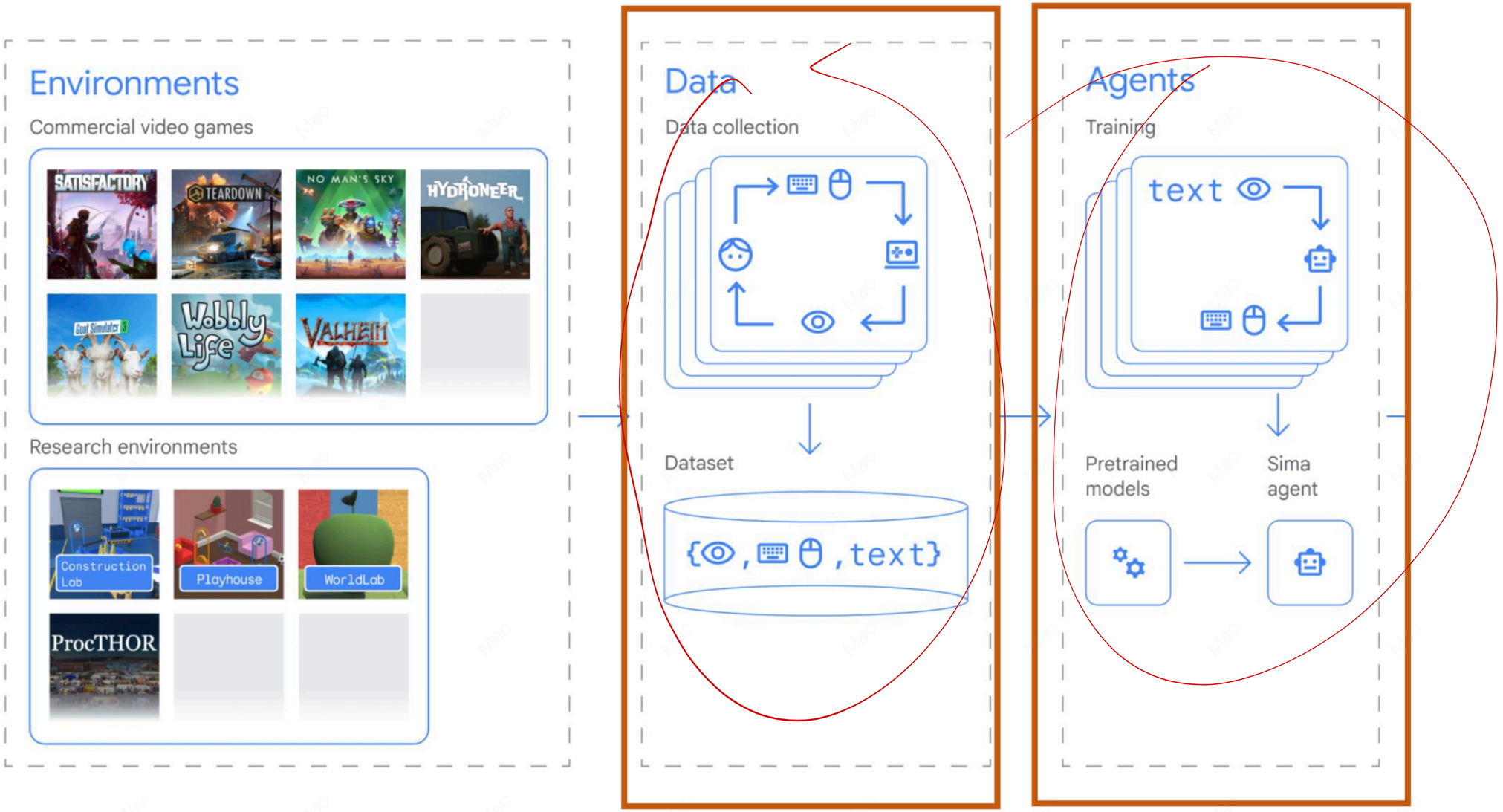
Supervised Finetuning

- Collect large amount of expert trajectories (e.g. from human annotation)

```
task_intent, [(obs_1, action_1), …,(obs_N, action_N)]
```

- Finetune the LLM with standard cross-entropy loss.

Supervised Finetuning



Supervised Finetuning

- Data hungry
- Cannot learn much from failed trajectories
  - a_1, a_2, a_3, … ,a_10 – Success
  - a_1, a_2, a_3, … ,a_10 – Fail (Wasted)
- Need human trajectory?
  - Data augmentation techniques

Reward

Create More Training Data

Open-ended Environments

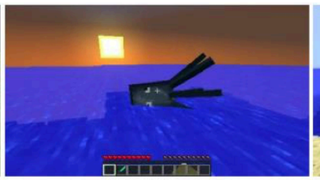
Craft Glass Bridge

Build Oak House

Make Ice Igloo

Combat Zombie

Fish Squid



Farm Sugar Cane

Find Ocean Monument

Explore Desert Temple

Treasure Hunt in End City

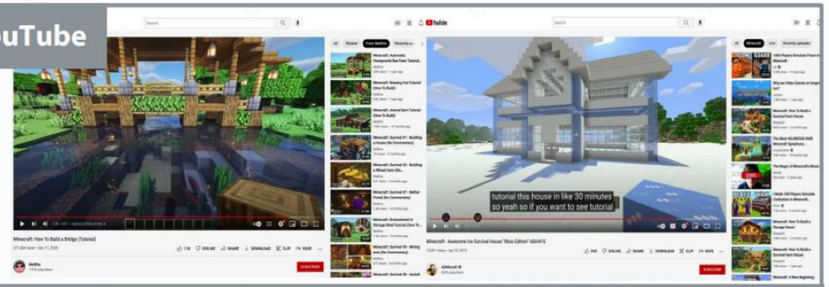
Generalist Agent

S_t

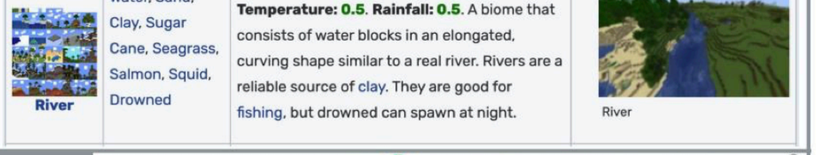
A_t

Internet-scale Knowledge Base

YouTube



Wiki



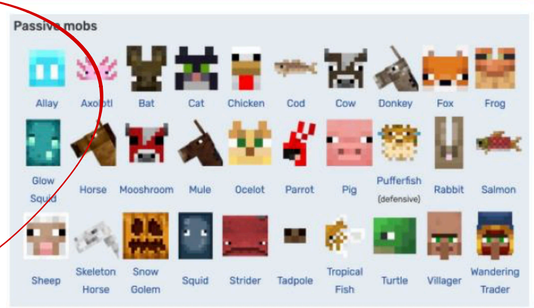
Reddit

Data Augmentation

- Continue pre-train on large amount of data automatically mined
- Even noisy, not clear trajectories, provide domain adaptation.

YouTube

Wiki



Name	Ingredients	Crafting recipe
Cake	Milk Bucket + Sugar + Egg + Wheat	
Golden Apple	Gold Ingot + Apple	

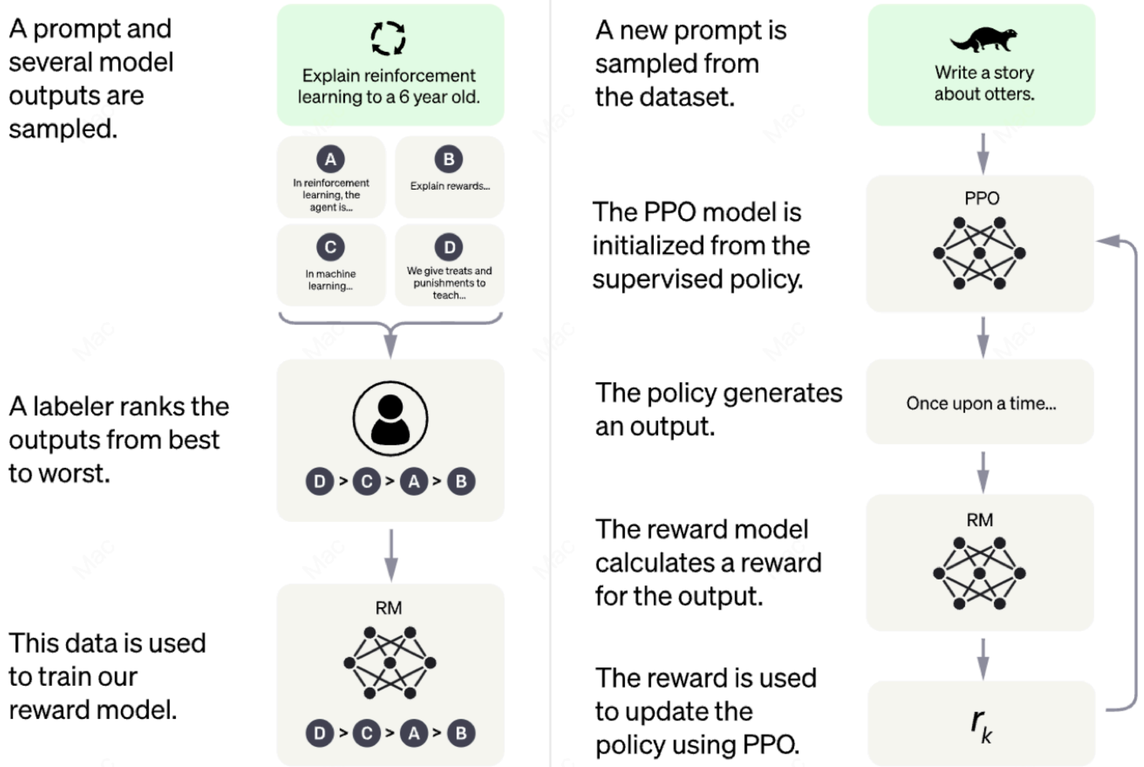
Reddit

MineDojo, Fan et al. 22’
Don’t Stop Pretraining, Gururangan et al., 20’

Reinforcement Learning

Lots of on-going research in this area!

Recall RLHF: Reinforcement Learning from Human Feedback:



RLVR

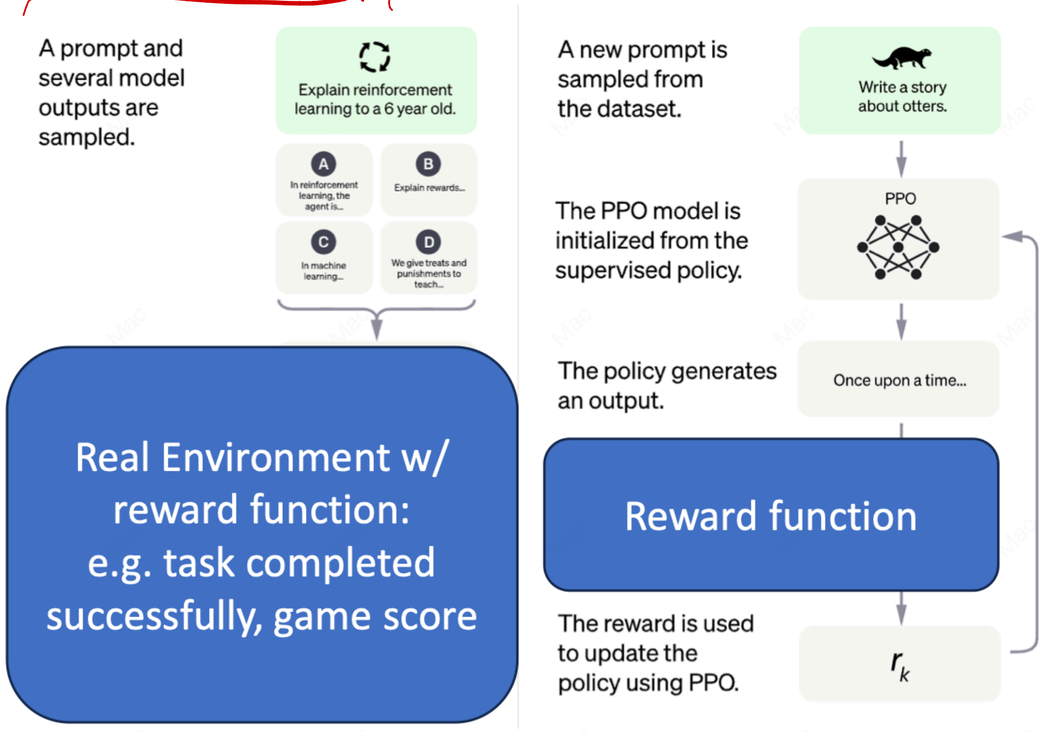
RLHF, Ouyang, et al. 22'

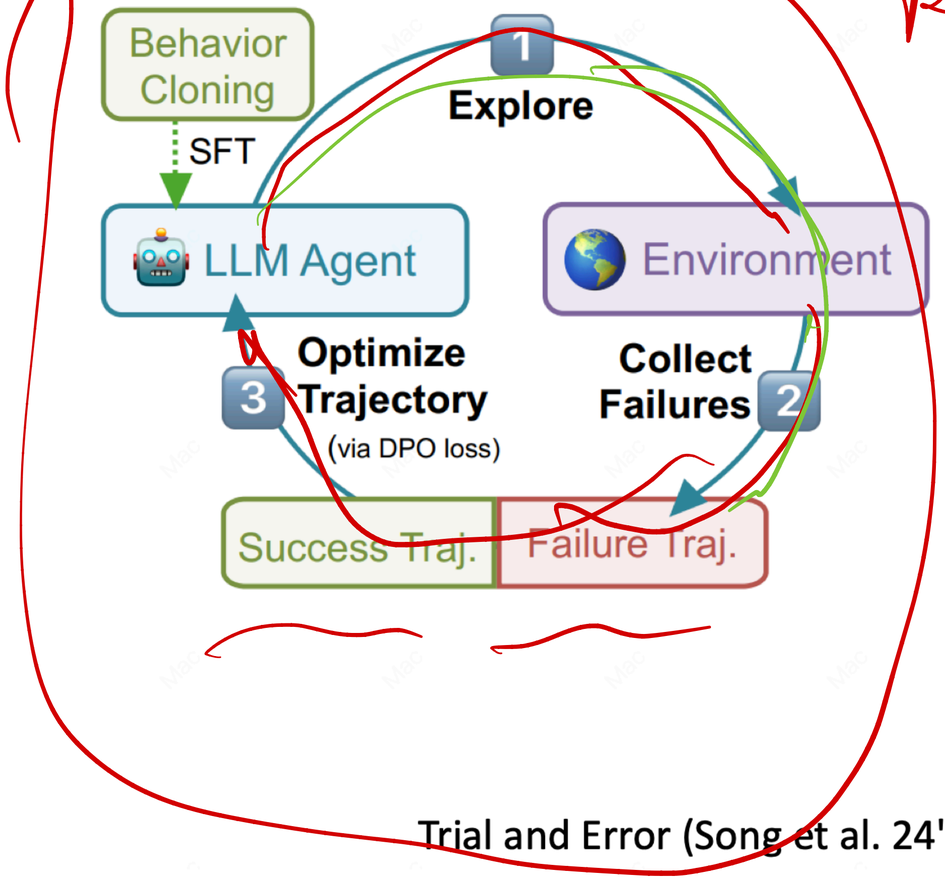
Reinforcement Learning

Compared to RLHF:

Given environment, *reward function*

(trajectory, reward) pairs without human

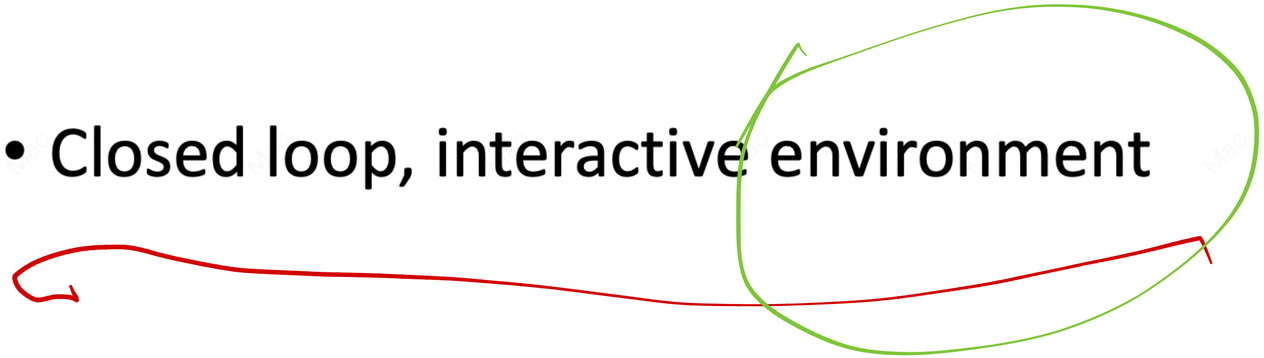




Trial and Error (Song et al. 24')

Reinforcement Learning

- Closed loop, interactive environment



Reinforcement Learning

- Closed loop, interactive environment

- Need good reward functions
  - What if the task success/fail is not easy to automatically assess?

Reinforcement Learning

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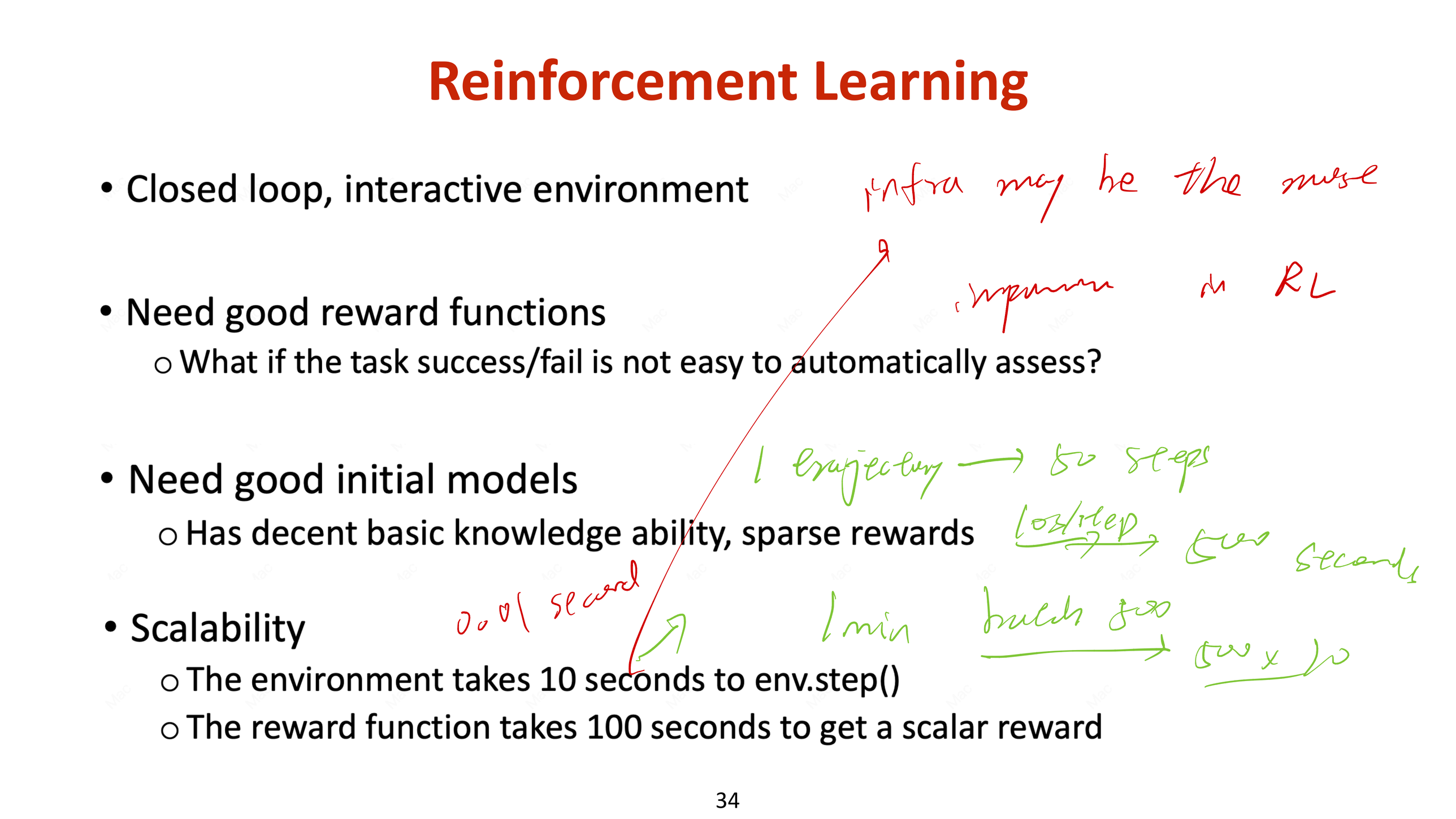
  - Has decent basic knowledge ability, sparse rewards

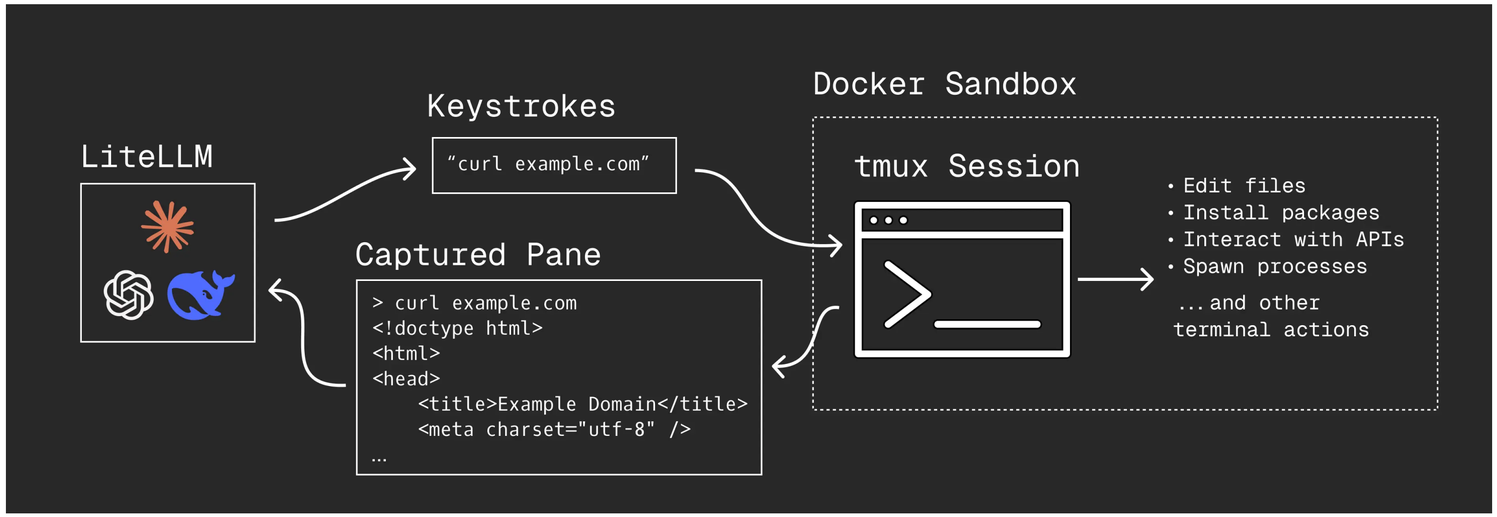
Reinforcement Learning

- Closed loop, interactive environment
- Need good reward functions
  - What if the task success/fail is not easy to automatically assess?
- Need good initial models
  - Has decent basic knowledge ability, sparse rewards
- Scalability
  - The environment takes 10 seconds to env.step()
  - The reward function takes 100 seconds to get a scalar reward



RL Environments

Environments and benchmarks typically come together



RL Environments

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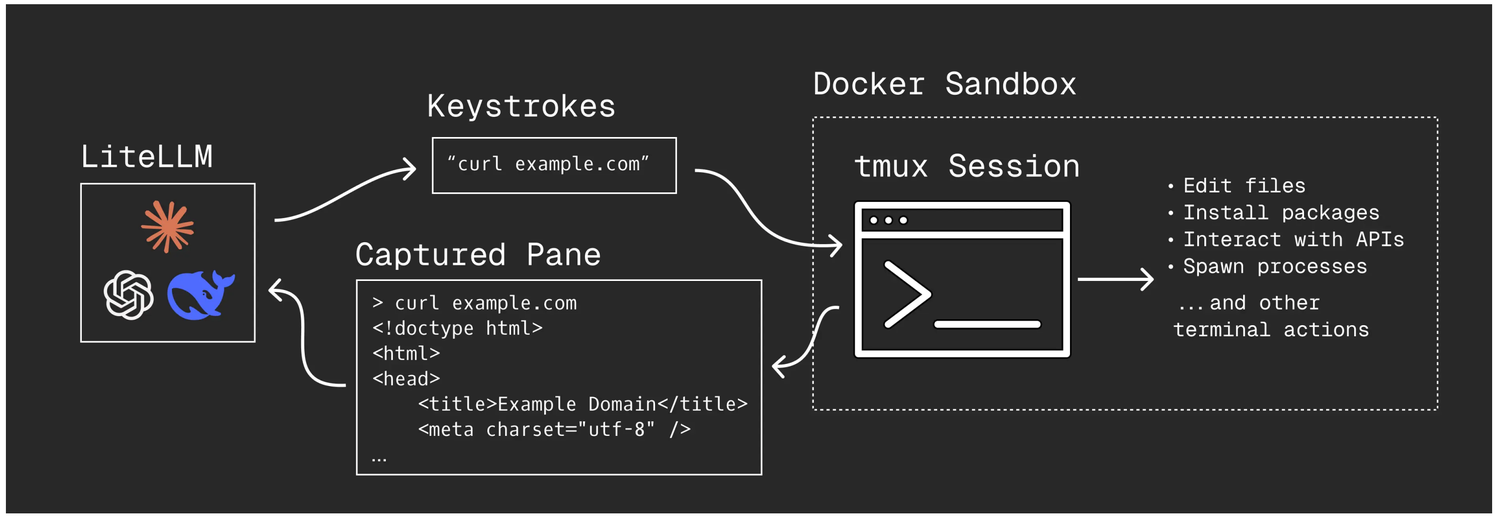
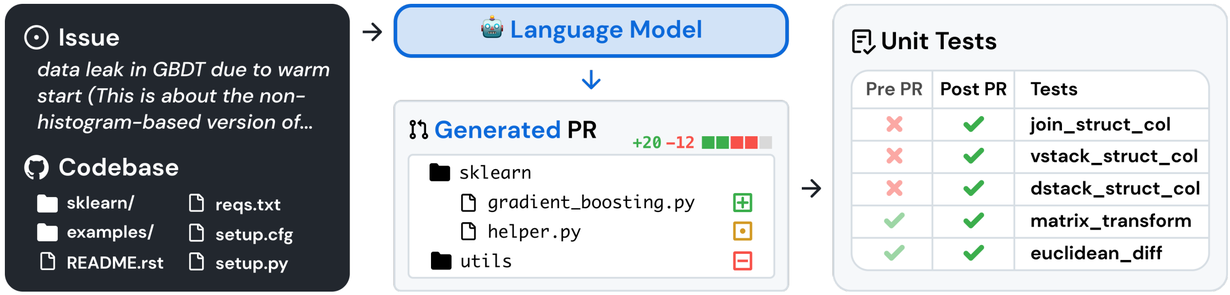
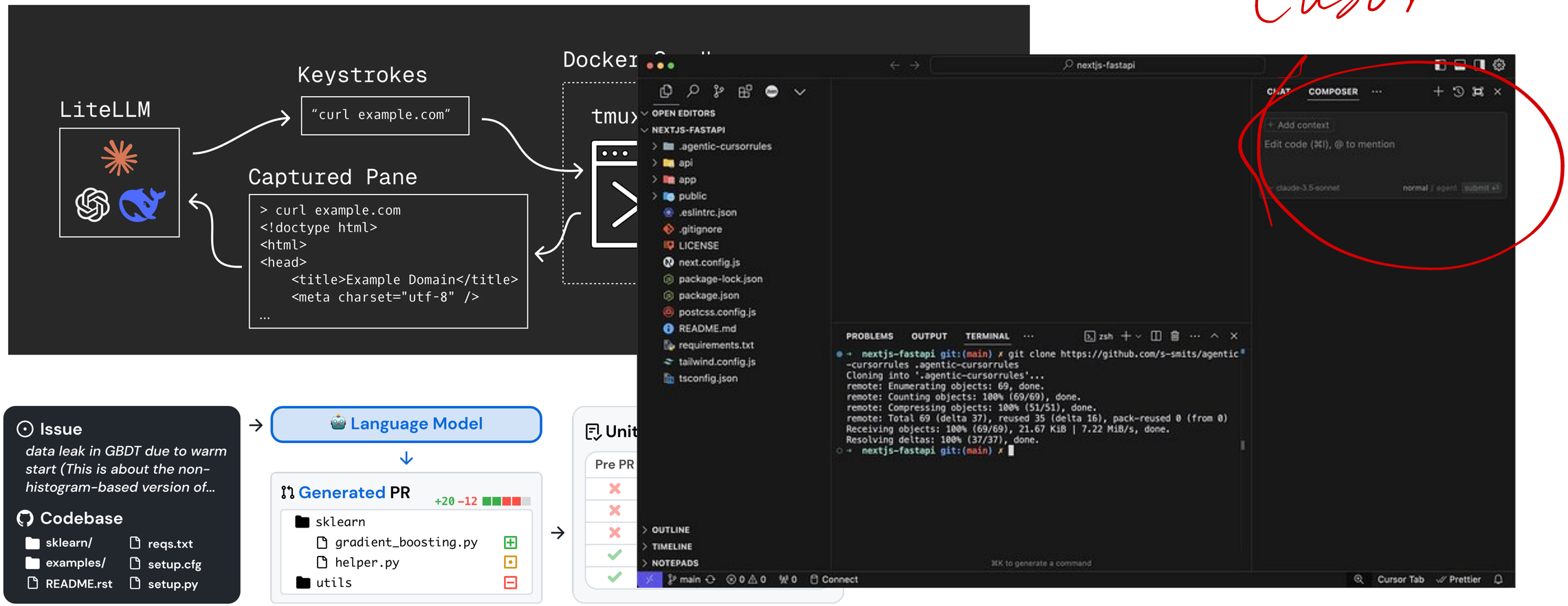




RL Environments

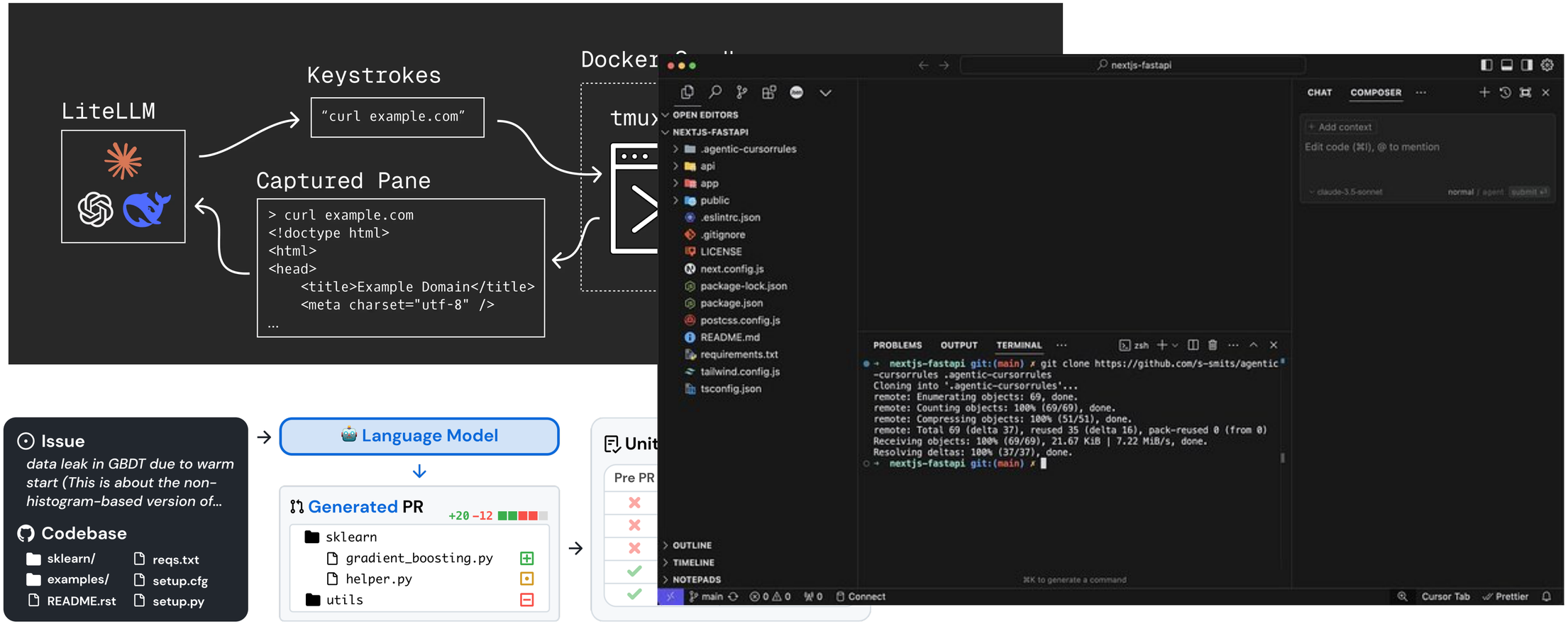
Environments and benchmarks typically come together



Cursor

RL Environments

Environments and benchmarks typically come together



Research and Products are really close nowadays, and we can directly RL in real, product-level environments

Thank You!