



Tool Use for Language Model Agents

How models turn token predictions into actions

Carnegie Mellon University
Language Technologies Institute

Graham Neubig
Language Technologies Institute



Basic idea

Tool definition

A tool is an interface through which a language model can invoke an external computer program.

Search

Calculator

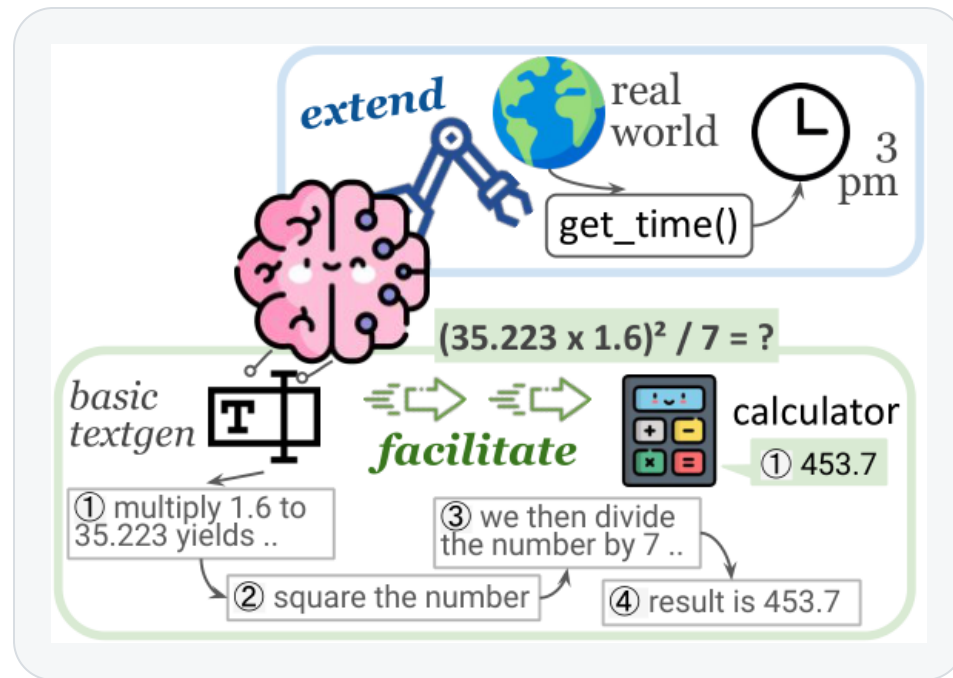
Browser

Python

API

The model proposes; external software decides whether and how to execute.

Benefits of tools



Extend

Access information or actions unavailable in the model's parameters.

Facilitate

Delegate operations external programs perform more reliably or efficiently.

Tool-use scenarios

Need	Example tool	Benefit
Current information	Search	Fresh evidence
Exact computation	Calculator or Python	Reliable execution
Private state	Account API	Authorized application data
External action	Browser or API	Changes the environment

Call tools only when their benefit outweighs latency, cost, failure, and risk.

Examples of tools

Building ChatGPT

What sorts of things can you help me do?

I can answer questions, find information, run code, create images, and complete specific workflows.

What calls are necessary?

Start from the abilities we want, then define a narrow interface for each kind of interaction.

Textual responses

```
finish(text)
```

Return the final text and stop the agent loop. This is a harness control action, not an external program.

What is the capital of Ghana?

CONTROL finish("Accra is the capital of
CALL Ghana.")

Accra is the capital of Ghana.

Information retrieval

```
search_web(query)
```

Retrieve information from the web.

What did CMU announce today?

**TOOL
CALL**

```
search_web("site:cmu.edu announced  
today")
```

**TOOL
RESULT**

Three matching news items...

CMU announced three items today...

Code execution

```
execute_code(code  
)
```

Run a program in an isolated environment and return its output.

What is the mean of 18, 23, 41, and 54?

**TOOL
CALL**

```
execute_code("sum([18,23,41,54])/4")
```

**TOOL
RESULT**

34.0

The mean is 34.

Image generation

```
generate_image(query)
```

Generate an image from a textual description.

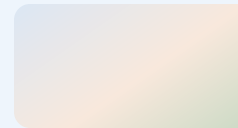
Create a watercolor robot studying in a library.

**TOOL
CALL**

```
generate_image("watercolor robot  
studying in a library")
```

**TOOL
RESULT**

generated_image.png



Here is the generated image.

Custom functions

```
create_grocery_cart(items)
```

Expose an application-specific capability through one typed call.

Make a cart with bananas, milk, and coffee.

**TOOL
CALL**

```
create_grocery_cart(["bananas", "milk",  
"coffee"])
```

**TOOL
RESULT**

Cart C17 · 3 items · \$31.42

I created a three-item cart totaling \$31.42.



Programmatic tool calling

Code as a meta-tool

build-in functions → tools

Q: The bakers baked 200 loaves of bread ...
How many loaves of bread did they have left?

LM The bakers started with 200 loaves. They
sold 93 in the morning ...The answer is 62.

```
loaves_baked, loaves_returned = 200, 6  
sold_morning, sold_afternoon = 93, 39  
answer = loaves_baked - loaves_sold_morning  
- loaves_sold_afternoon + loaves_returned
```

CodeLM

external libraries → tools

Q: The table shows how many... What is the
max number of vacation days across years?

Year	2013	2014	2015
Vacation days	23	18	11

```
import pandas as pd  
df = pd.DataFrame({"Year": [2013, 2014, 2015],  
"Vacation days": [23, 18, 11]})  
max_days = df["Vacation days"].max()
```

CodeLM

utility functions → tools

Q: Who is wearing the dress?



```
dress_box = locate_objects(image, "dress")  
dress_region = crop_region(image, dress_box)  
answer = visual_qa(dress_region,  
question="Who is wearing the dress?")
```

CodeLM

Code composes control flow, libraries, and multiple operations in one action.

Programmatic composition

Instruction: Determine the most cost-effective country to purchase the smartphone model "CodeAct 1". The countries to consider are the USA, Japan, Germany, and India.

Available APIs

[1] lookup_rates(country: str) -> (float, float)
[2] convert_and_tax(price: float, exchange_rate: float, tax_rate: float) -> float

[3] estimate_final_price(converted_price: float, shipping_cost: float) -> float
[4] lookup_phone_price(model: str, country: str) -> float
[5] estimate_shipping_cost(destination_country: str) -> float

LLM Agent using [Text/JSON] as Action

Think I should calculate the phone price in USD for each country, then find the most cost-effective country.

Action Text: lookup_rates, Germany
JSON: {"tool": "lookup_rates", "country": "Germany"}

Environment 1.1, 0.19

Action Text: lookup_phone_price, CodeAct 1, Germany
JSON: {"tool": "lookup_phone_price", "model": "CodeAct 1", "country": "Germany"}

Environment 700

Action Text: convert_and_tax, 700, 1.1, 0.19
JSON: {"tool": "convert_and_tax", "price": 700, "exchange_rate": 1.1, "tax_rate": 0.19}

Environment 916.3

[... interactions omitted (look up shipping cost and calculate final price) ...]

Action Text: lookup_rates, Japan
JSON: {"tool": "lookup_rates", "country": "Japan"}

[... interactions omitted (calculate final price for all other countries)...]

Response The most cost-effective country to purchase the smartphone model is Japan with price 904.00 in USD.

Fewer Actions Required!

CodeAct: LLM Agent using [Code] as Action

Think I should calculate the phone price in USD for each country, then find the most cost-effective country.

Action

```
countries = ['USA', 'Japan', 'Germany', 'India']
final_prices = {}

for country in countries:
    exchange_rate, tax_rate = lookup_rates(country)
    local_price = lookup_phone_price("xAct 1", country)
    converted_price = convert_and_tax(
        local_price, exchange_rate, tax_rate
    )
    shipping_cost = estimate_shipping_cost(country)
    final_price = estimate_final_price(converted_price, shipping_cost)
    final_prices[country] = final_price

most_cost_effective_country = min(final_prices, key=final_prices.get)
most_cost_effective_price = final_prices[most_cost_effective_country]
print(most_cost_effective_country, most_cost_effective_price)
```

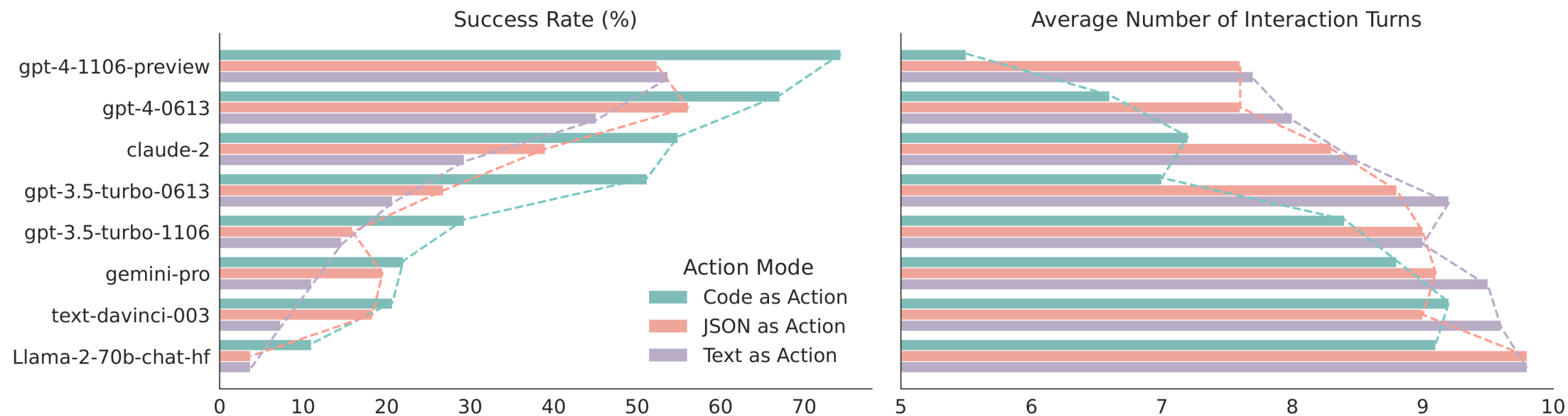
Environment 1.1, 0.19

Response The most cost-effective country to purchase the smartphone model is Japan with price 904.00 in USD.

Control & Data Flow of Code
Simplifies Complex Operations

Re-use `min` Function from Existing
Software Infrastructures (Python library)

CodeAct results



In the displayed subset, code had the best success rate for **8/8** models.

Code used the fewest turns for **7/8**; across all 17 models, both counts are **12/17**.

Code is a high-power tool

Expressive

Loops · variables · libraries

Good for multi-step data manipulation and composition.

Harder to constrain

Broad action space

Validation is less precise than for a narrow typed function.

Higher impact

Files · network · processes

Use sandboxing, resource limits, permissions, and audit logs.



Mechanics of providing tools

Tool calls as tokens

Text continuation

The weather is sunny.

Tool continuation

```
<tool_call>  
get_weather( ... )
```

The model requests an action. The harness executes it.

Quick review: messages become model input

API messages

system Be concise.

user Weather in Pittsburgh?

assistant I need current data.

chat template



Qwen input sequence

```
<|im_start|>system
```

```
Be concise.<|im_end|>
```

```
<|im_start|>user
```

```
Weather in Pittsburgh?<|im_end|>
```

```
<|im_start|>assistant
```

```
I need current data.<|im_end|>
```

Roles structure the API; the template serializes one model-input sequence.

Tools add structure to the request

Tool definition

```
{
  "type": "function",
  "function": {
    "name": "get_weather",
    "parameters": {
      "type": "object",
      "properties": {"city": {"type": "string"}},
      "required": ["city"]
    }
  }
}
```

API request

```
response =
client.chat.completions.create(
    model=model,
    messages=messages,
    tools=[weather_tool],
)
```

The harness sends messages and tool schemas; the template exposes both to the model.

Definition in, tool call out

Prompt contains

```
<tools>
{"name": "get_weather", ...}
</tools>
```

model



Model emits

```
<tool_call>
{"name": "get_weather",
 "arguments": {"city": "Pittsburgh"}}
</tool_call>
```

The model emits the call content; the API response attaches a unique call ID.

Same tool call, different model protocols

Qwen 3.8

Function + parameter tags

```
<|im_start|>assistant  
<tool_call>  
<function=get_weather>  
<parameter=city>  
Pittsburgh  
</parameter>  
</function>  
</tool_call><|im_end|>
```

Mistral Small 4

Control token + call ID

```
[ TOOL_CALLS ] [ { "name":  
  "get_weather",  
  "arguments": { "city":  
    "Pittsburgh" }, "id":  
    "abc123xyz" } ] </s>
```

DeepSeek V3.2

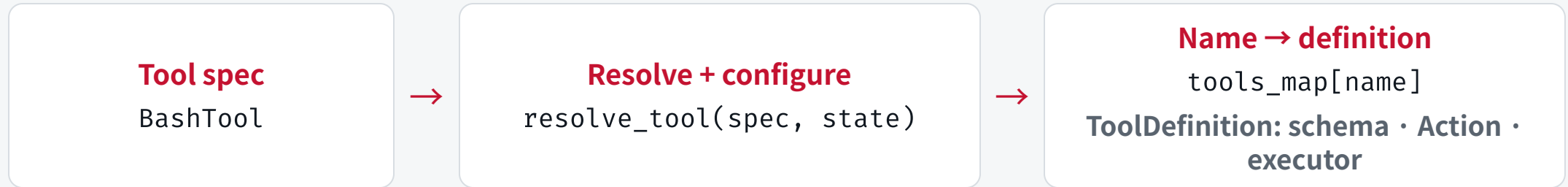
DSML invocation block

```
< | DSML | function_calls>  
< | DSML | invoke  
  name="get_weather">  
< | DSML | parameter  
  name="city"  
  string="true">Pittsburgh<  
/ | DSML | parameter>  
</ | DSML | invoke>  
</ | DSML | function_calls>
```

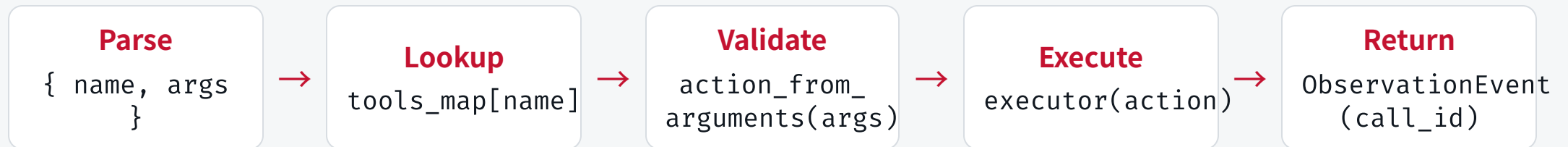
One schema; model-specific serialization and parsing.

How OpenHands dispatches a tool call

1 Register at initialization



2 Dispatch each model call



Results return by call ID

Assistant tool call

```
{  
  "id": "call_123",  
  "name": "get_weather",  
  "arguments": {"city":  
    "Pittsburgh"}  
}
```



Tool-result message

```
{  
  "role": "tool",  
  "tool_call_id": "call_123",  
  "content": "72°F · sunny"  
}
```

`tool_call_id` matches results to calls, including parallel calls.



Constrained decoding

Malformed tool calls

Model output

```
{"name": "get_weather",  
  "arguments": {"city": "Pittsburgh"}}
```



Missing }

The harness cannot parse it.

Tool-call constraints

Syntax

valid JSON

Shape

expected fields

Types

city is a string

Values

units is C or F

Constraints ensure form—not truth, permissions, tool choice, or task success.

JSON Schema

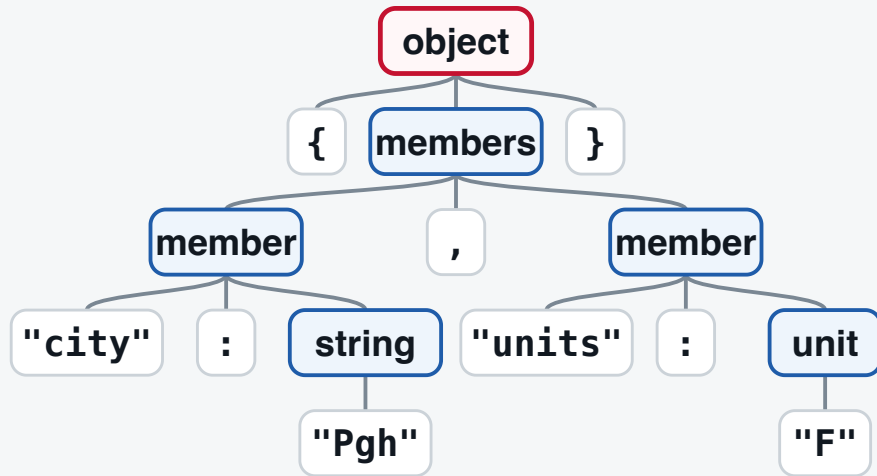
- Vocabulary for describing JSON data
- Types, required fields, allowed values
- Machine-readable validation rules

```
{  
  "type": "object",  
  "properties": {  
    "city": {"type": "string"},  
    "units": {"enum": ["C", "F"]}  
  },  
  "required": ["city"],  
  "additionalProperties": false  
}
```

Schema-valid vs. schema-invalid

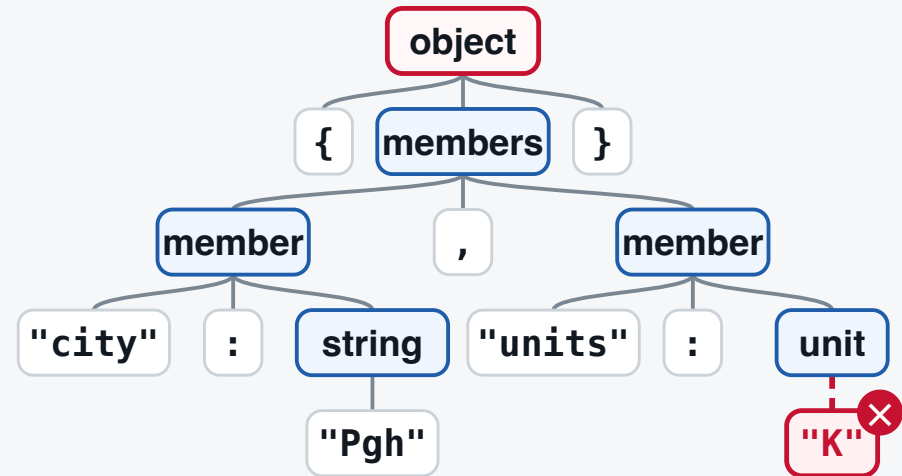
Schema-valid

```
{"city": "Pgh", "units": "F"}
```



Schema-invalid

```
{"city": "Pgh", "units": "K"}
```



Both are JSON; only "F" derives from `unit → "C" | "F"`.

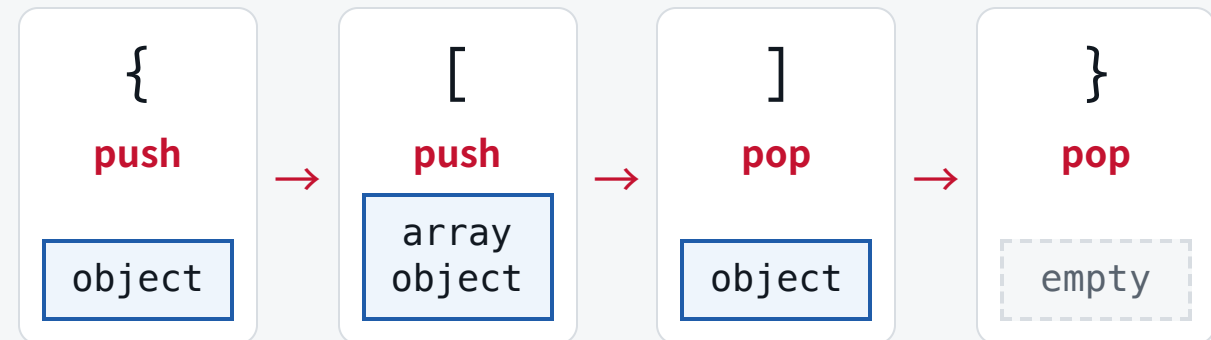
A pushdown automaton adds a stack

Finite control



State records the local position in a grammar rule.

Stack memory

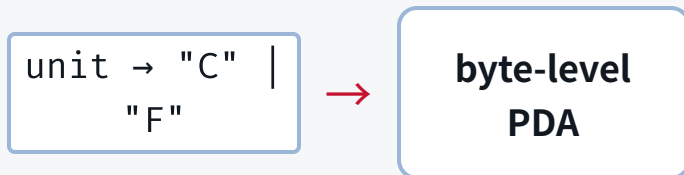


The stack remembers arbitrarily deep nesting.

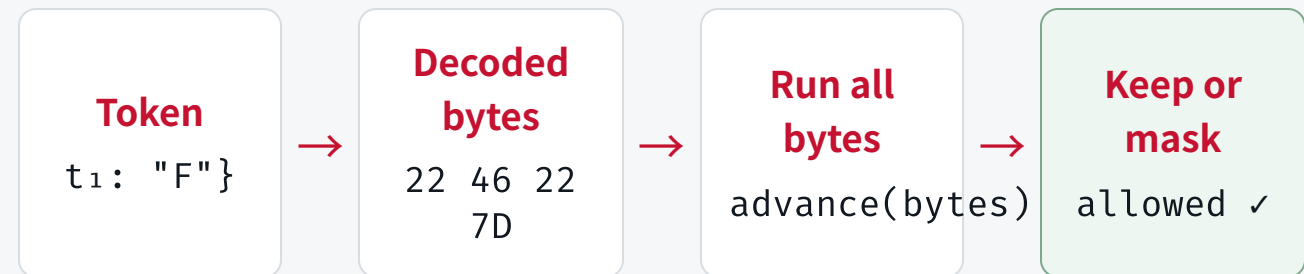
State tracks the current rule; the stack remembers where nested rules return.

Grammar checking happens below tokenization

Compile once



Check every candidate token



A token may cross several grammar terminals—or end partway through one—so token boundaries cannot be treated as grammar boundaries.

Example: cached token-mask generation

1 · Parse the prefix

Advance persistent PDA stacks over the bytes already emitted.

2 · Fetch cached decisions

The stack-top node indexes precomputed validity for context-independent tokens.

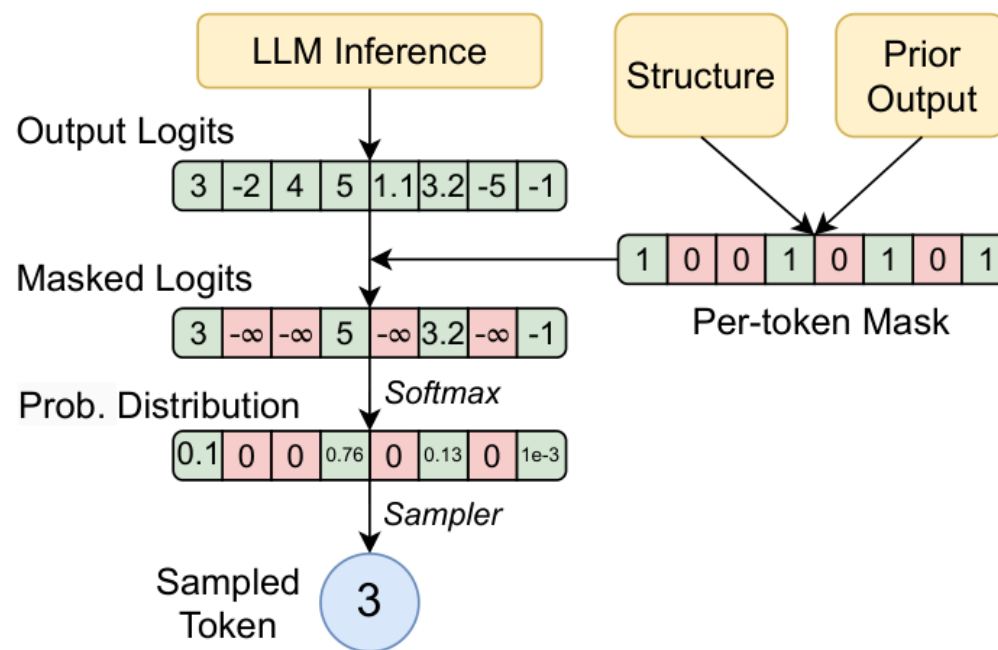
3 · Check the minority

Run context-dependent candidate tokens against the full stack; union results across matching stacks.

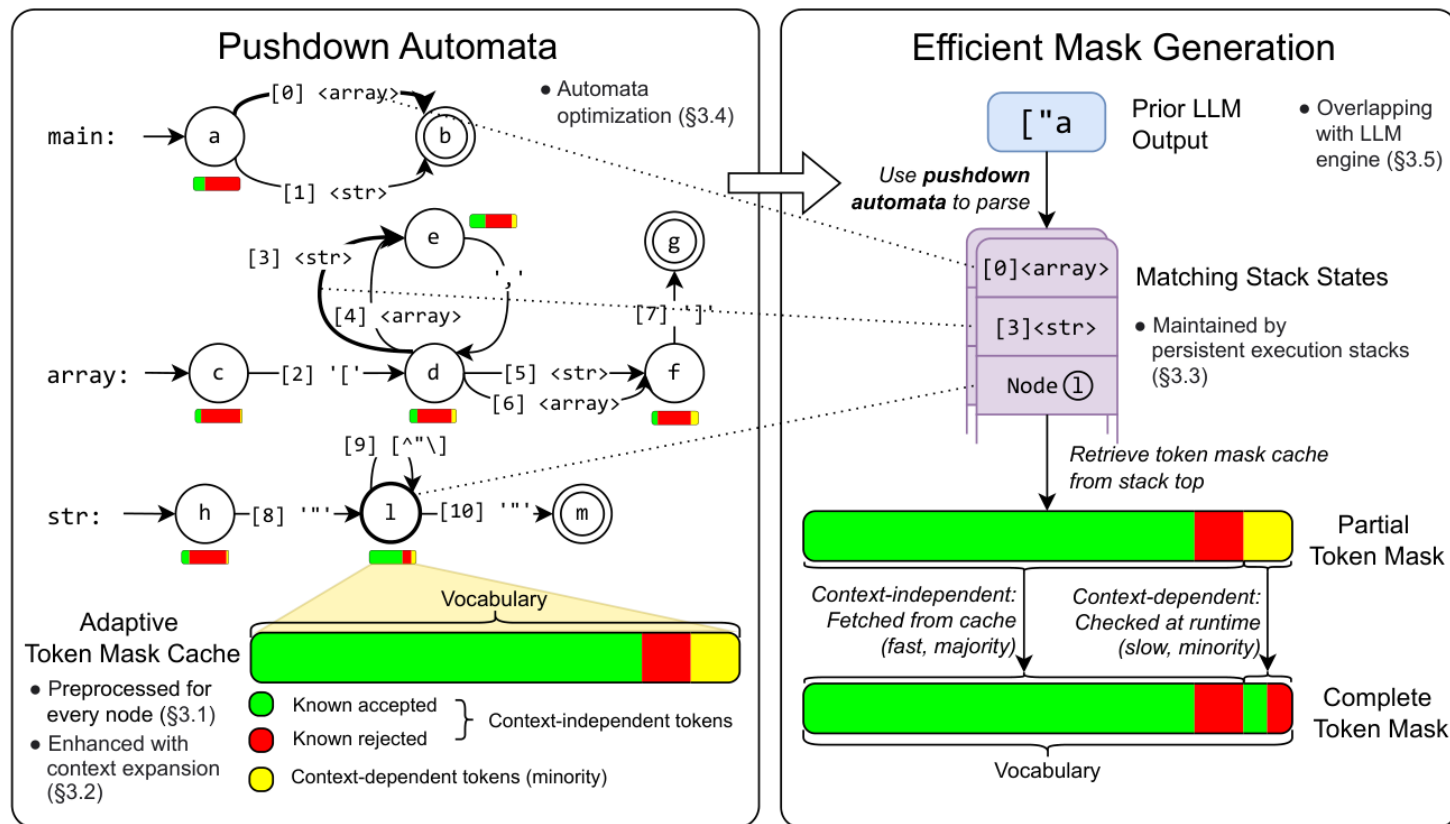
4 · Mask and continue

Combine the decisions, mask the logits, sample a token, and update the PDA stacks.

Token masking



Case study: where the speedup comes from



Caching handles most tokens; persistent stacks support branching; CPU work overlaps GPU inference.



REST API Calling

Libraries expose in-process APIs

```
# weather_lib.py
from typing import Literal
from pydantic import BaseModel

class Weather(BaseModel):
    summary: str
    temperature: float

def get_weather(
    city: str,
    units: Literal["C", "F"] = "F",
) -> Weather:
    return provider.lookup(city, units)
```

Caller and function share one process

Python supplies the name, arguments, types, and return type.

Not remotely callable yet

A network client still needs an address, protocol, serialization, and authentication.

A library API is a typed programming interface—not a network service.

REST APIs expose functions over HTTP

```
# api.py
from typing import Annotated, Literal
from fastapi import FastAPI, Security
from fastapi.security import APIKeyHeader
from weather_lib import Weather, get_weather

app = FastAPI(title="Weather API")
key_header = APIKeyHeader(name="X-API-Key")

@app.get("/weather", operation_id="get_weather")
def weather(
    city: str,
    key: Annotated[str, Security(key_header)],
    units: Literal["C", "F"] = "F",
) -> Weather:
    verify(key)
    return get_weather(city, units)
```

GET /weather

city=Pittsburgh

units=F

Header: X-API-Key

Response: Weather as JSON

FastAPI binds the library function to a REST endpoint and documents its API-key header.

REST API servers publish OpenAPI descriptions

```
{
  "paths": {"/weather": {"get": {
    "operationId": "get_weather",
    "parameters": [
      {"name": "city", "in": "query", "required": true,
       "schema": {"type": "string"}},
      {"name": "units", "in": "query",
       "schema": {"type": "string", "enum": ["C", "F"], "default": "F"}}
    ],
    "security": [{"APIKeyHeader": []}]
  }}},
  "components": {"securitySchemes": {"APIKeyHeader": {
    "type": "apiKey", "in": "header", "name": "X-API-Key"
  }}}
}
```

OpenAPI describes the HTTP operation; embedded **JSON Schema** describes its values.

Coding agents often call REST APIs with curl

```
curl -sS -G https://weather.example/weather \  
  --data-urlencode "city=Pittsburgh" \  
  --data-urlencode "units=F" \  
  -H "X-API-Key: $WEATHER_API_KEY"
```

1 · Read the API description

Select the operation and required parameters.

2 · Construct the command

The shell expands the environment variable; curl sends HTTP.

3 · Limit the credential

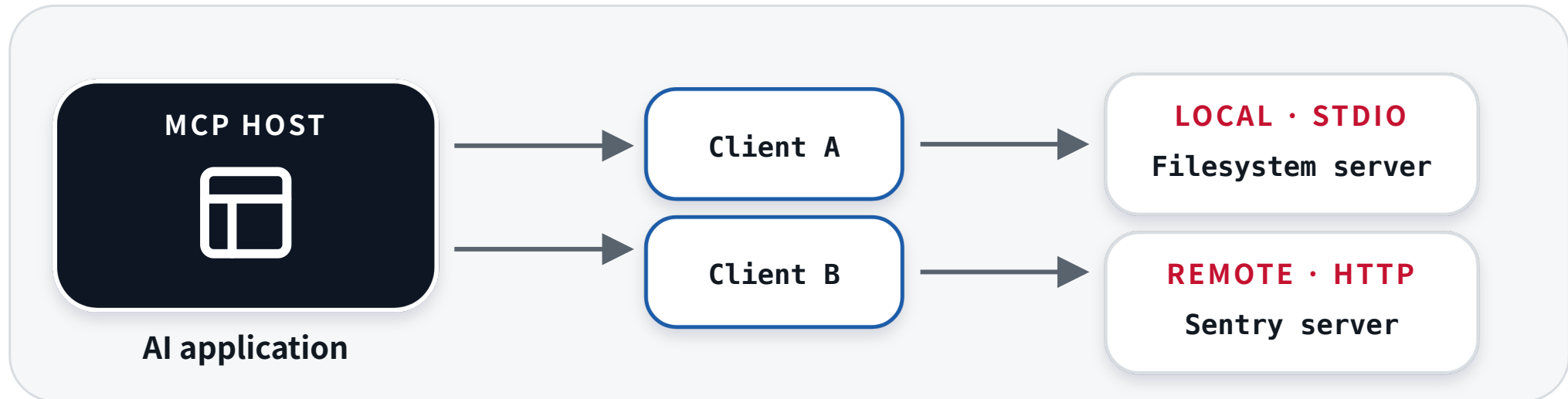
A coding agent with shell access may also read or misuse that secret.

Direct REST access is simple, but the agent's shell receives the API credential.



MCP

MCP connects a host to servers



MCP is an alternative agent-facing interface—not a requirement for calling REST APIs.

FastMCP projects OpenAPI operations as MCP tools

```
import httpx2
from fastmcp import FastMCP

spec = httpx2.get(
    "https://weather.example/openapi.json"
).json()

mcp = FastMCP.from_openapi(
    openapi_spec=spec,
    client=httpx2.AsyncClient(
        base_url="https://weather.example"
    ),
    name="Weather MCP",
)
```

OpenAPI operation

GET /weather



MCP tool

get_weather(city, units)

By default, FastMCP converts each OpenAPI route into a discoverable MCP tool.

Start MCP with separate credentials

```
import os, httpx2
from fastmcp import FastMCP
from fastmcp.server.auth.providers.jwt import StaticTokenVerifier

upstream = httpx2.AsyncClient(
    base_url="https://weather.example",
    headers={"X-API-Key": os.environ["UPSTREAM_API_KEY"]})
mcp_auth = StaticTokenVerifier(tokens={
    os.environ["MCP_API_KEY"]: {"client_id": "course-agent"}})

mcp = FastMCP.from_openapi(
    openapi_spec=spec, client=upstream,
    name="Weather MCP", auth=mcp_auth)
mcp.run(transport="http", port=8001)
```

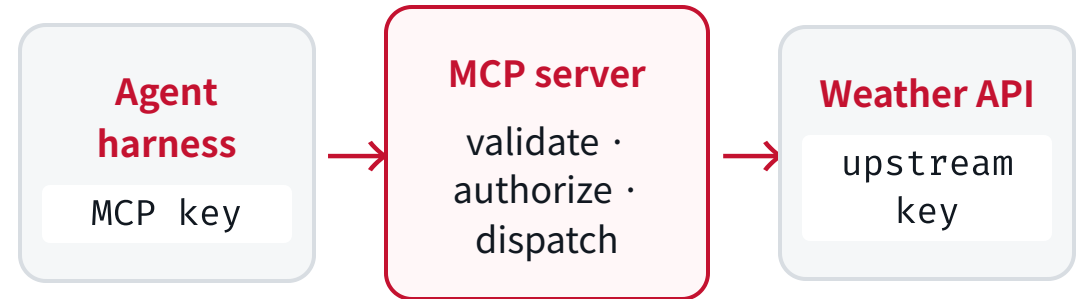
`UPSTREAM_API_KEY` authorizes API calls; `MCP_API_KEY` protects the MCP endpoint.

Static tokens are for teaching/development; production deployments should verify JWTs or use OAuth.

The MCP client uses its own API key

```
import os
from fastmcp import Client

async with Client(
    "https://mcp.example/mcp",
    auth=os.environ["MCP_API_KEY"],
) as client:
    tools = await client.list_tools()
    result = await client.call_tool(
        "get_weather",
        {"city": "Pittsburgh", "units": "F"},
    )
```



Credential brokering: the server accepts one credential and uses a different credential upstream. The model sees neither secret.

Separate credentials let the MCP server mediate access instead of forwarding its upstream secret.

REST APIs and MCP: shared schemas, different contracts

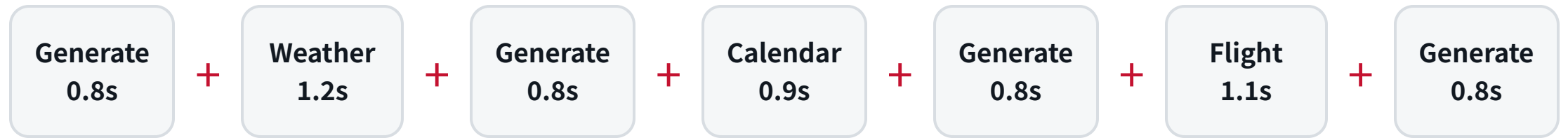
	OpenAPI / HTTP API	MCP
Shared	Names, descriptions, and JSON Schema for structured inputs	
Discovery	Fetch an OpenAPI document	Call <code>tools/list</code> at runtime
Invocation	HTTP verb + path + parameters	<code>tools/call</code> over an MCP transport
Authentication	Client authenticates to the API	Client authenticates to MCP; upstream auth is separate
Scope	Describes HTTP operations	Also supports resources, prompts, and extensions

OpenAPI describes a web API; MCP standardizes how an AI host discovers and invokes capabilities.



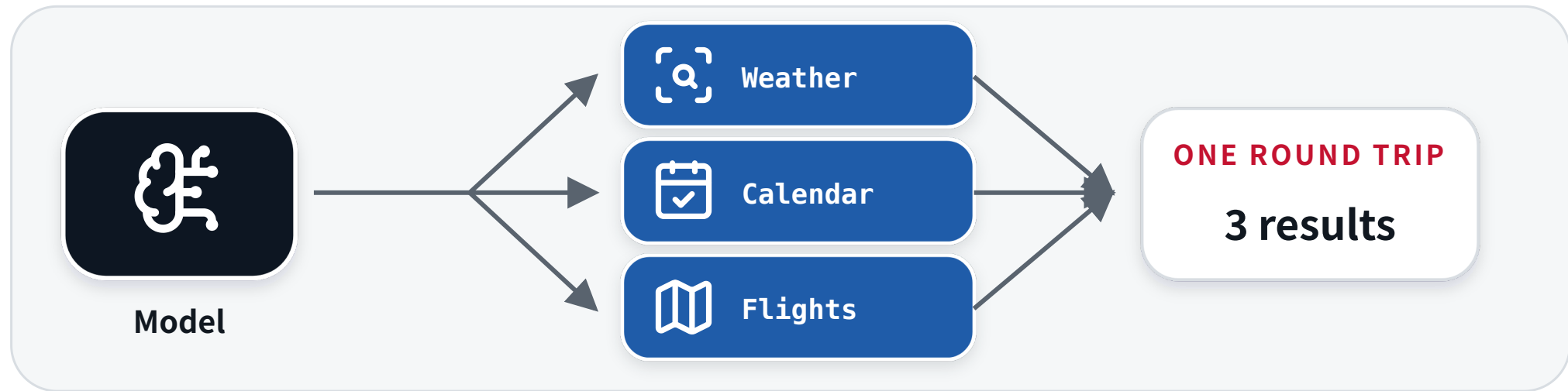
Orchestrating multiple calls

Serial tool-call cost



≈ 6.4 seconds

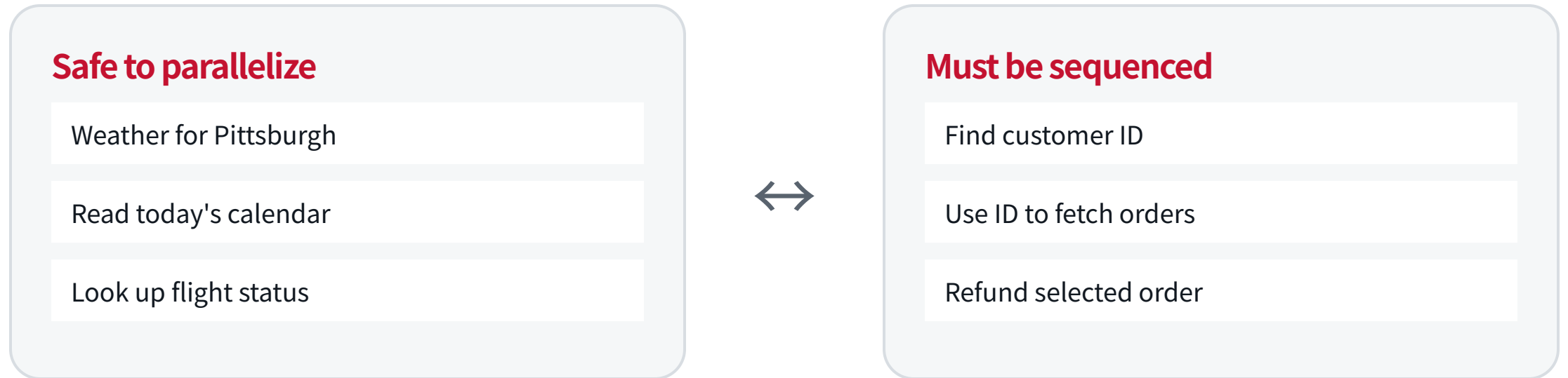
Parallel tool calls



Independent calls can share one generation and one wait.

Two generation phases plus the slowest tool: $2 \times 0.8 + \max(1.2, 0.9, 1.1) \approx \mathbf{2.8 \text{ seconds}}$.

Parallelize only without dependencies



Parallelize only independent, safely concurrent calls.

Concurrent execution

```
async def execute(call):  
    args = json.loads(call.arguments)  
    value = await TOOLS[call.name](**args)  
    return call.call_id, value  
  
results = await asyncio.gather(  
    *(execute(call) for call in function_calls),  
    return_exceptions=True,  
)
```

Preserve call IDs when results finish out of order.



Evaluating tool use

Berkeley Function Calling Leaderboard

Single turn

simple · multiple · parallel · multiple-parallel

Multi-turn

base · missing function · missing parameter · long context

Agentic

web search · memory

Robustness

hallucination measurement · format sensitivity

Evaluate the whole stack

Level	Question	Example metric	Execution?	Typical failure
Selection	Right tool?	Precision / recall	No	Missing or extra call
Arguments	Right values?	AST / schema match	No	Wrong field or value
Trajectory	Right order?	Sequence success	Usually	Bad dependency
Task	Goal achieved?	End-to-end success	Yes	Plausible wrong answer

Quality has operational dimensions

Efficiency

Latency · calls · tokens · cost

A correct agent can still be unusably slow or expensive.

Reliability

Timeouts · retries · partial failure

Report task success under realistic provider behavior.

Safety

Policy · permissions · side effects

Test adversarial outputs and consequential actions.

Operational tool failures

Model

wrong tool · bad arguments ·
ignores result

Harness

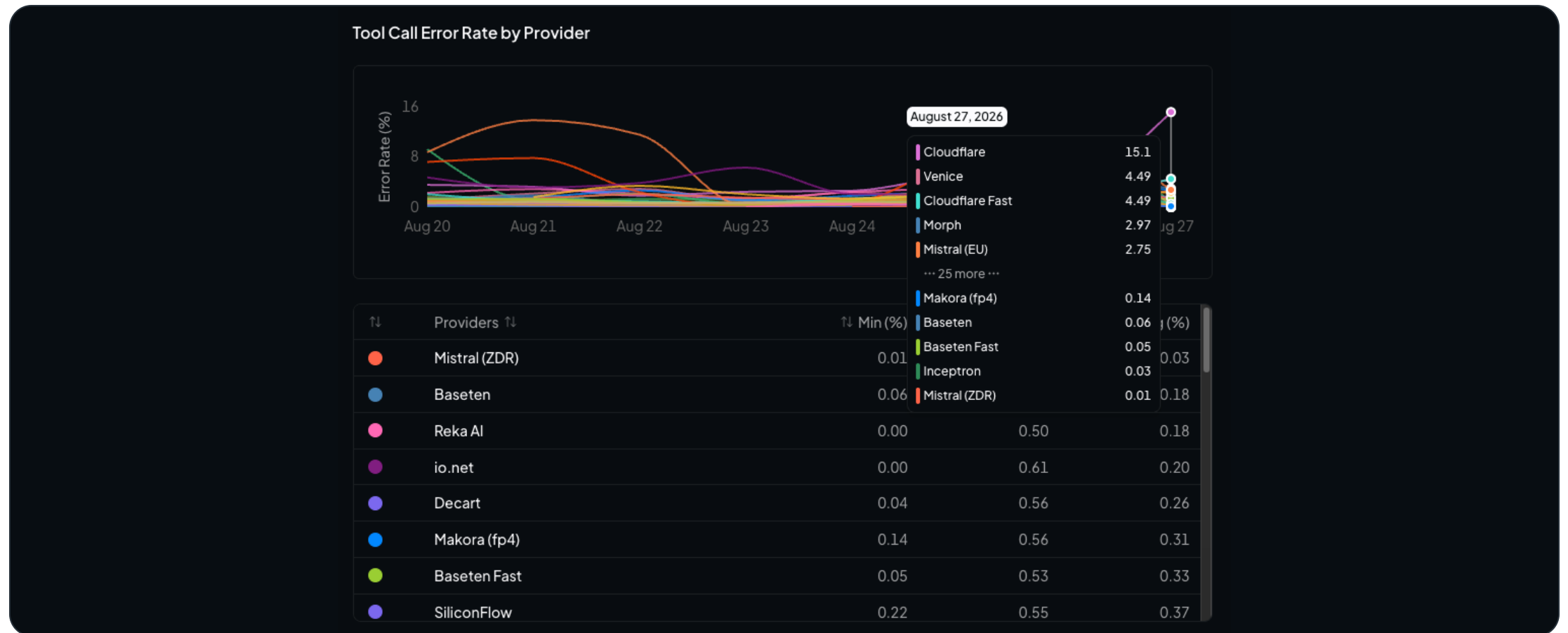
parse · auth · validation · ID
mismatch

Provider or tool

timeout · rate limit · execution
error

Production evaluation needs benchmark accuracy and operational failure rates.

Provider tool-call error rates

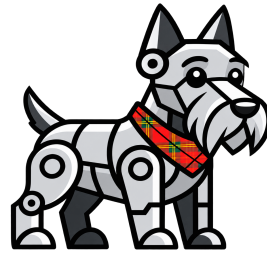




Takeaways

Tool use is a layered system

- 1 **Capabilities:** tools add retrieval, execution, generation, and application actions.
- 2 **Mechanics:** schemas enter the prompt; model protocols emit calls; harnesses validate, dispatch, and match results by ID.
- 3 **Constraints:** JSON Schema and grammar masks guarantee form—not semantic correctness.
- 4 **Interfaces:** direct REST calls and MCP are alternative ways to expose capabilities and manage credentials.
- 5 **Systems:** orchestrate dependencies and concurrency; evaluate selection, arguments, outcomes, cost, and operational failures.



Thank you, Questions?

Next Class: Agent Capabilities 2 — Context Management for Long-Context LLMs