

Tool Use and Function Calling

Week 3: Extending LLMs with External Capabilities

PhD Course in Agentic Artificial Intelligence

Bloom's Taxonomy Levels

- **Remember:** Define function calling, MCP (Model Context Protocol), tool augmentation
- **Understand:** Explain how LLMs learn to use external tools
- **Apply:** Implement tool-using agents with OpenAI and Anthropic APIs
- **Analyze:** Compare different tool integration approaches
- **Evaluate:** Assess tool selection strategies and error handling
- **Create:** Design custom tools and integrate into agent workflows

Tool

use transforms LLMs from text generators into action-taking agents.

LLM Limitations

- Knowledge cutoff (can't access current information)
- No computation ability (unreliable at math)
- Can't interact with external systems
- Hallucinate when uncertain

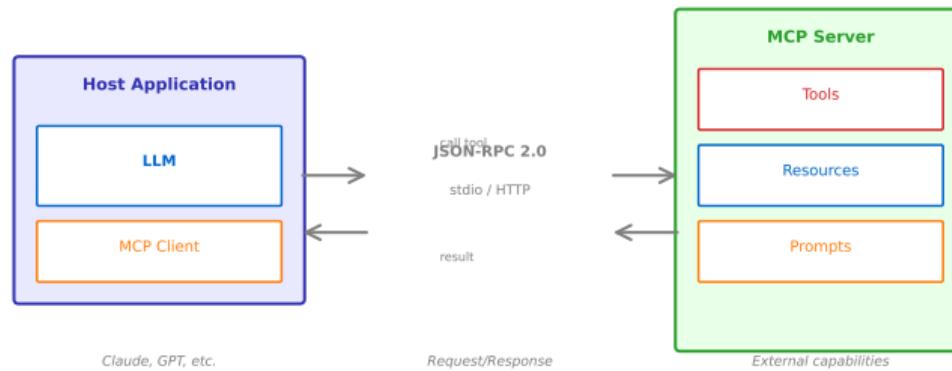
Tools Enable

- Real-time information retrieval (web search, APIs)
- Precise computation (calculators, code execution)
- System interaction (databases, file systems)
- Grounded responses (verified facts)

(Schick et al., 2023): LLMs can learn to use tools autonomously.

Model Context Protocol (MCP)

Model Context Protocol (MCP) Architecture



is Anthropic's open protocol for connecting LLMs to external tools.

MCP

Three Primitives

- **Tools:** Functions the LLM can call (search, calculate, etc.)
- **Resources:** Data sources (files, databases, APIs)
- **Prompts:** Reusable prompt templates

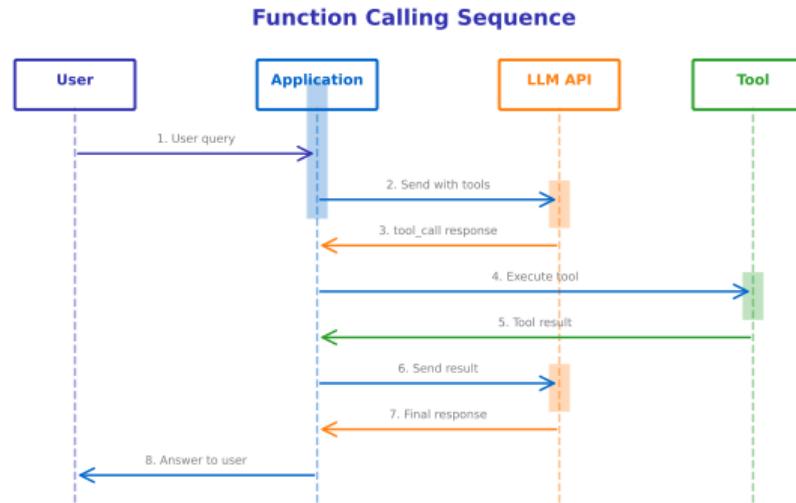
Transport Layer

- JSON-RPC 2.0 (structured messaging) over stdio or HTTP
- Request/response pattern with typed schemas
- Supports streaming for long-running operations

Key Advantage: Standardized protocol across different LLM providers

enables tool portability: write once, use with any LLM.

Function Calling Sequence



LLM decides when and which tool to call based on the query.

The

Tool Definition (JSON Schema = typed structure)

```
{"type": "function", "function": {"name": "get_weather",  
    "description": "Get weather for a location",  
    "parameters": {"type": "object",  
        "properties": {"location": {"type": "string"}},  
        "required": ["location"]}}}
```

Key Points

- Clear descriptions help LLM choose correct tool
- JSON Schema for parameter validation
- LLM returns structured tool_calls array

tool descriptions are critical for reliable tool selection.

Good

Claude Tool Definition

```
{"name": "get_weather",
  "description": "Get weather for a location",
  "input_schema": {"type": "object",
    "properties": {"location": {"type": "string"}},
    "required": ["location"]}}
```

Differences from OpenAI

- Uses input_schema instead of parameters
- Returns tool_use content blocks
- Supports tool_choice for forcing specific tools

and OpenAI have similar but not identical APIs.

Tool Selection Strategies

Selection Approaches

- **Auto:** LLM decides when/which tool (default)
- **Required:** Force at least one tool call
- **Specific:** Force a particular tool
- **None:** Disable tool use

Best Practices

- Start with “auto” and monitor selection quality
- Use “required” when you know a tool is needed
- Provide 3-5 tools max for reliable selection
- Include negative examples in descriptions

many tools degrade selection accuracy – keep toolsets focused.

Too

Common Failure Modes

- Tool not found or invalid parameters
- Tool execution timeout
- External API failure
- Malformed tool response

Recovery Strategies

- **Retry with backoff:** For transient failures
- **Fallback tools:** Alternative tools for same task
- **Graceful degradation:** Inform user of limitation
- **Self-correction:** Let LLM try different approach

error handling is essential for production agents.

API-Bank (Li et al., 2023)

- Benchmark with 73 APIs across 3 levels of complexity
- Tests tool selection, parameter extraction, composition
- GPT-4 achieves 80%+ on single-tool tasks

ToolLLM (Qin et al., 2024)

- 16,000+ real-world APIs from RapidAPI
- Trains open models for tool use
- Introduces ToolBench for evaluation

Gorilla (Patil et al., 2023)

- LLM fine-tuned for API documentation
- Reduces hallucination in API parameters

shows tool use is learnable but challenging to scale.

Resea

Security Considerations

Risks

- **Prompt injection:** Malicious input that hijacks LLM behavior
- **Parameter injection:** Malicious inputs to tool parameters
- **Privilege escalation:** Tools with more access than intended
- **Data exfiltration:** Tools sending sensitive data externally

Mitigations

- Validate and sanitize all tool inputs
- Implement principle of least privilege
- Use allowlists for external connections
- Log all tool calls for audit

use introduces new attack surfaces – security is critical.

Tool

Building Custom Tools

Tool Design Checklist

- ① Clear, specific name (verb + noun)
- ② Detailed description with examples
- ③ Minimal required parameters
- ④ Typed parameters with constraints
- ⑤ Structured return format

Example: Search Tool

- Name: `search_web`
- Description: “Search the web for current information. Use for recent events, facts to verify, or when knowledge might be outdated.”
- Parameters: `query` (string, required)
- Returns: structured JSON with title, snippet, url

`tool design = clear intent + minimal friction.`

Good

This Week

- Anthropic MCP Documentation: docs.anthropic.com/mcp

Supplementary

- Schick et al. (2023). “Toolformer.” arXiv:2302.04761
- Li et al. (2023). “API-Bank.” arXiv:2304.08244
- Qin et al. (2024). “ToolLLM.” arXiv:2307.16789
- Patil et al. (2023). “Gorilla.” arXiv:2305.15334

documentation is required; papers provide research context.

Summary and Key Takeaways

Key Concepts

- **Function Calling:** Structured tool invocation by LLMs
- **MCP:** Open protocol for tool integration
- **Tool Design:** Clear names, descriptions, typed parameters
- **Security:** Validate inputs, minimize privileges

Key APIs

- OpenAI: tools parameter with JSON Schema
- Anthropic: tools with `input_schema`

Next Week

- Planning and Reasoning
- Reflexion: Learning from mistakes

transform LLMs from passive responders to active agents.

Tools