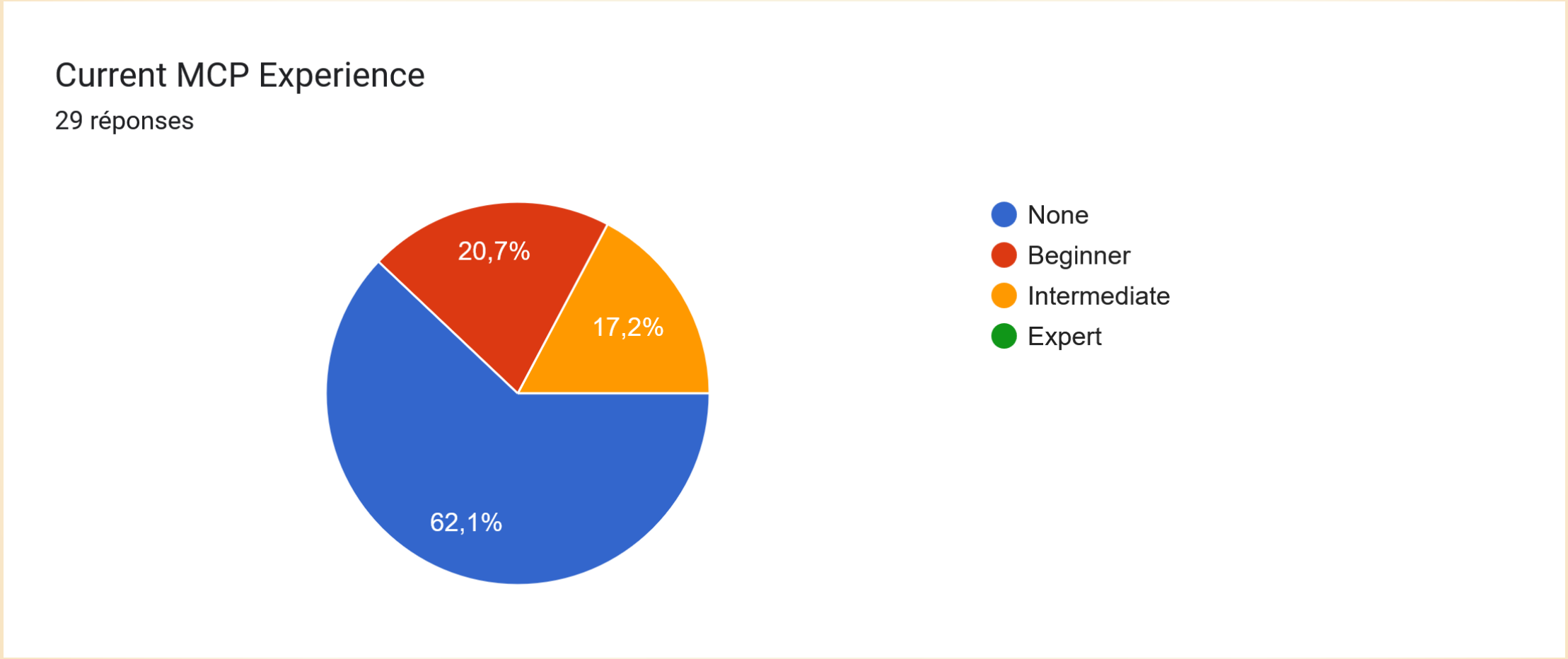
Cracking Shells

MCP servers for Scientific Applications

JACOPIN Eliott – RIKEN BDR BIC

RIKEN Hatchathon – 2025/08/28 – 29

MCP Experience



Schedule

<table>
<tr><th></th><th colspan="2">28/08</th><th>29/08</th></tr>
<tr><td>09:00</td><td colspan="2"></td><td rowspan="2">Workgroups Track Day 2</td></tr>
<tr><td>09:30</td><td colspan="2">Reception
(Get name tags, collecting fees for lunch & diner sessions,
getting all setup)</td></tr>
<tr><td>10:00</td><td rowspan="2">Workgroups Track Day 1</td><td rowspan="2">Beginner Track Part 1</td><td>Coffee and small snacks</td></tr>
<tr><td></td><td>Workgroups Track Day 2</td></tr>
<tr><td>12:00-13:00</td><td colspan="2">Lunch</td><td>Lunch</td></tr>
<tr><td>13:00-15:00</td><td></td><td>Beginner Track Part 2</td><td>Demonstrations & Presentations</td></tr>
<tr><td></td><td colspan="2">Coffee and small snacks</td><td>END</td></tr>
<tr><td>15:30</td><td colspan="2" rowspan="2">Workgroups Track Day 1</td><td rowspan="3"></td></tr>
<tr><td></td></tr>
<tr><td>18:00-20:00</td><td colspan="2">Diner Session</td></tr>
</table>

Beginner Track

1. Introduction presentation
   - What is MCP?
   - MCP for scientific applications
2. Setting up and using MCP servers
   - Use case of knowledge extraction from papers to knowledge graph
3. Implementing your own MCP servers
   - Simple arithmetic MCP server
4. More advanced MCP features
   - LLM sampling, logging, progress report, prompts, resources

Workgroup Tracks

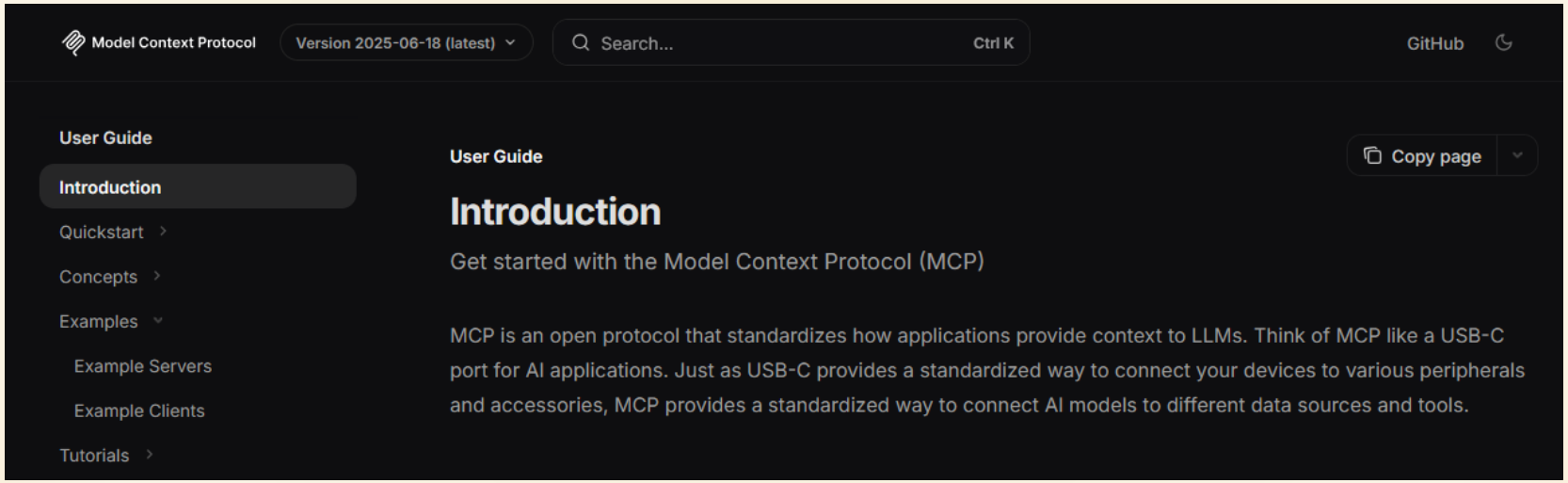
- Collaborative inside and in-between groups
- The goal is to achieve something and share with the group
  - Code
  - Best practices/failures
  - → Small report/code on https://github.com/CrackingShells/mcp-hackathon-fall-2025
  - → A 10min slides/demonstration tomorrow

What is MCP?

Model Context Protocol

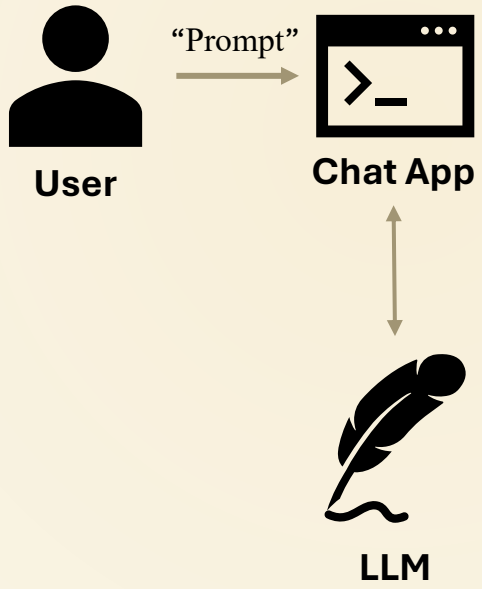
Origin

- Model Context Protocol (MCP)
- Created by Anthropic for their models
- Aims to become a standard in to connect LLMs to Software
- Made open source on November 2024

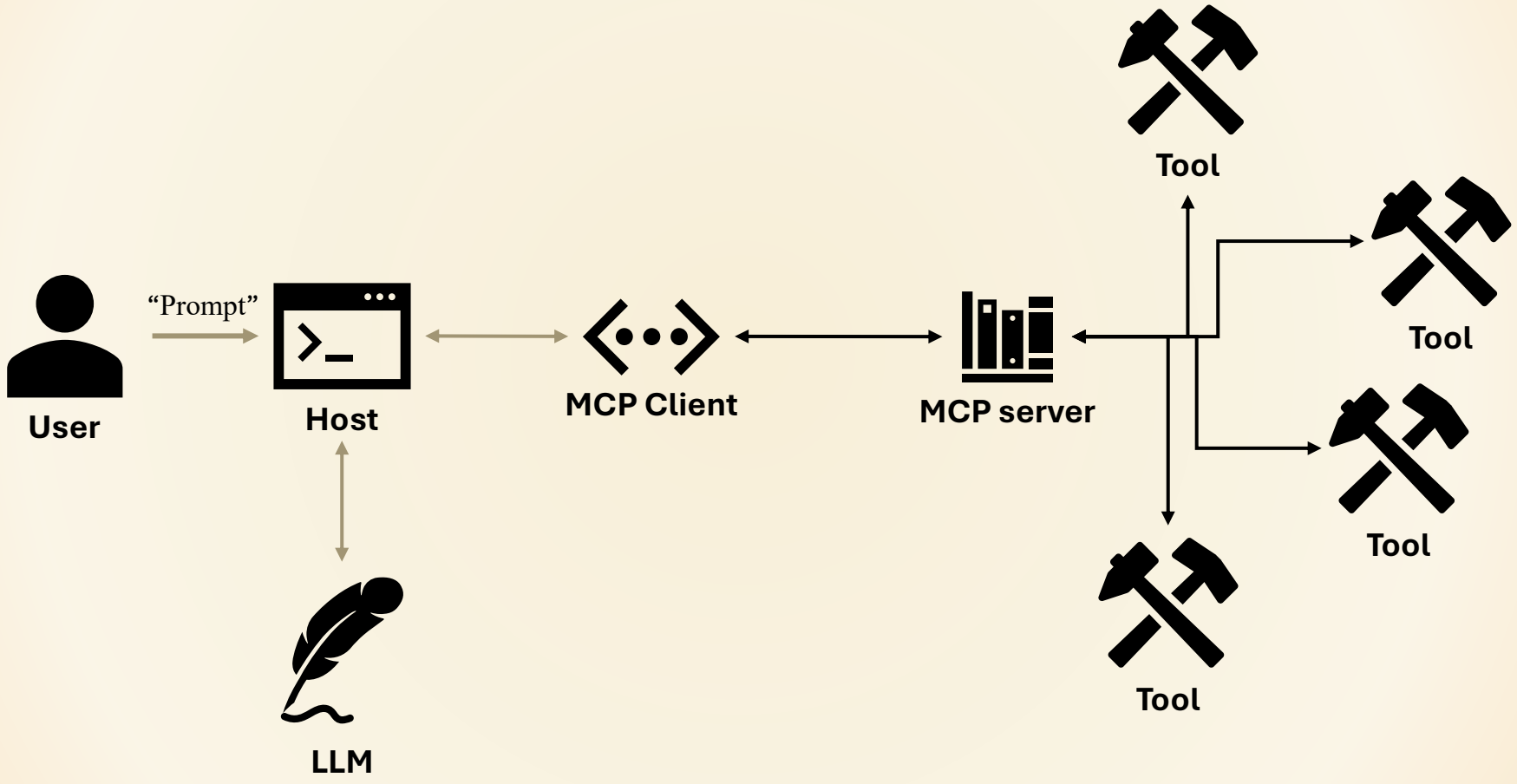


https://modelcontextprotocol.io/introduction

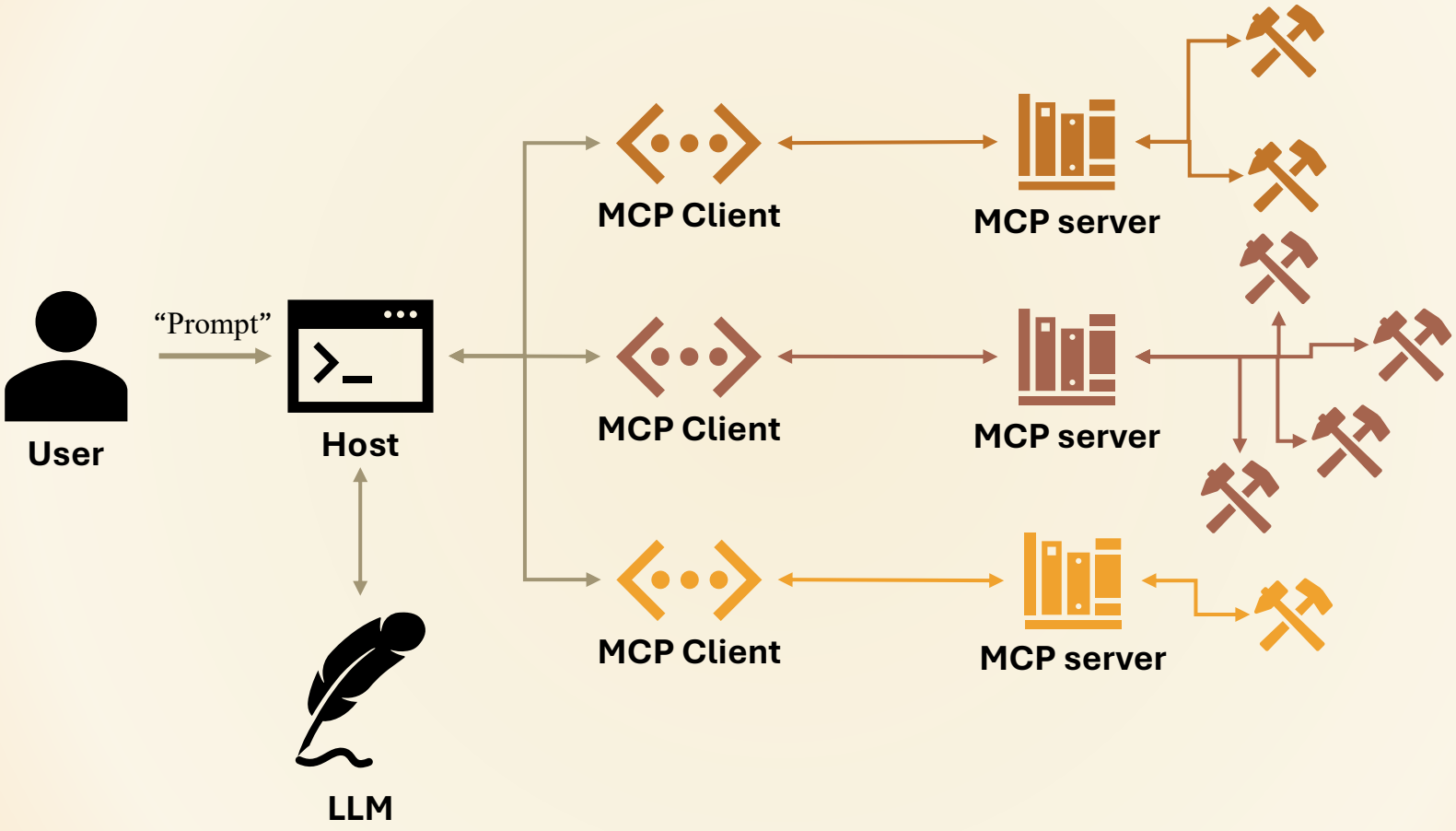
Architecture: basic chat app



Architecture: MCP Host - Client - Server



Architecture: as many servers as we want



MCP servers are easy to create

Let's create a simple MCP server that exposes a calculator tool and some data:

```python
# server.py
from mcp.server.fastmcp import FastMCP

# Create an MCP server
mcp = FastMCP("Demo")


# Add an addition tool
@mcp.tool()
def add(a: int, b: int) -> int:
    """Add two numbers"""
    return a + b


# Add a dynamic greeting resource
@mcp.resource("greeting://{name}")
def get_greeting(name: str) -> str:
    """Get a personalized greeting"""
    return f"Hello, {name}!"
```

Just a few lines.

https://github.com/modelcontextprotocol/python-sdk

MCP Ecosystem for Science

Making deployment of MCP servers easy

https://github.com/CrackingShells

“Products” on Cracking Shells

A package manager for MCP servers

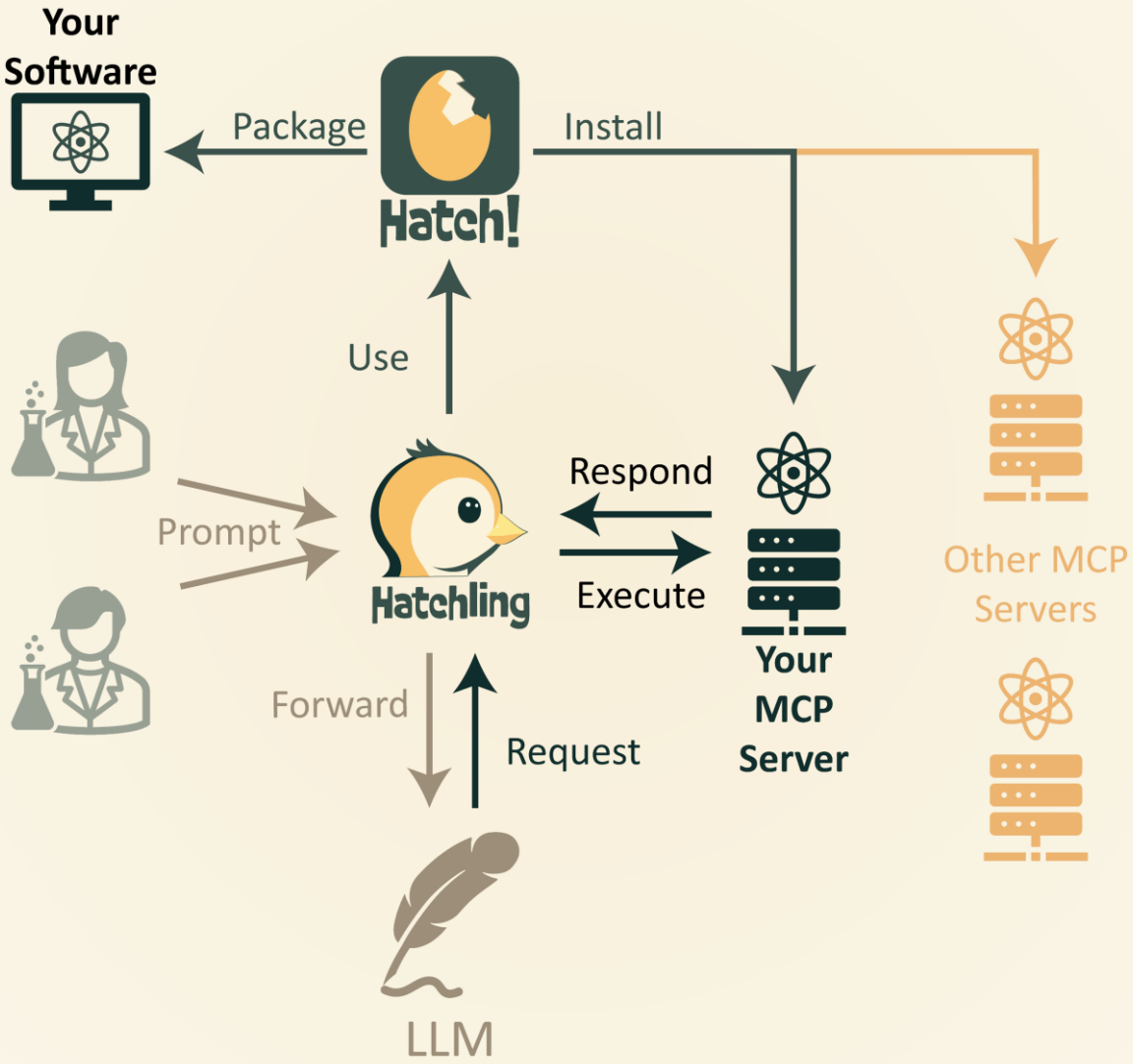
https://github.com/CrackingShells/Hatch

Chat Engine + CLI frontend

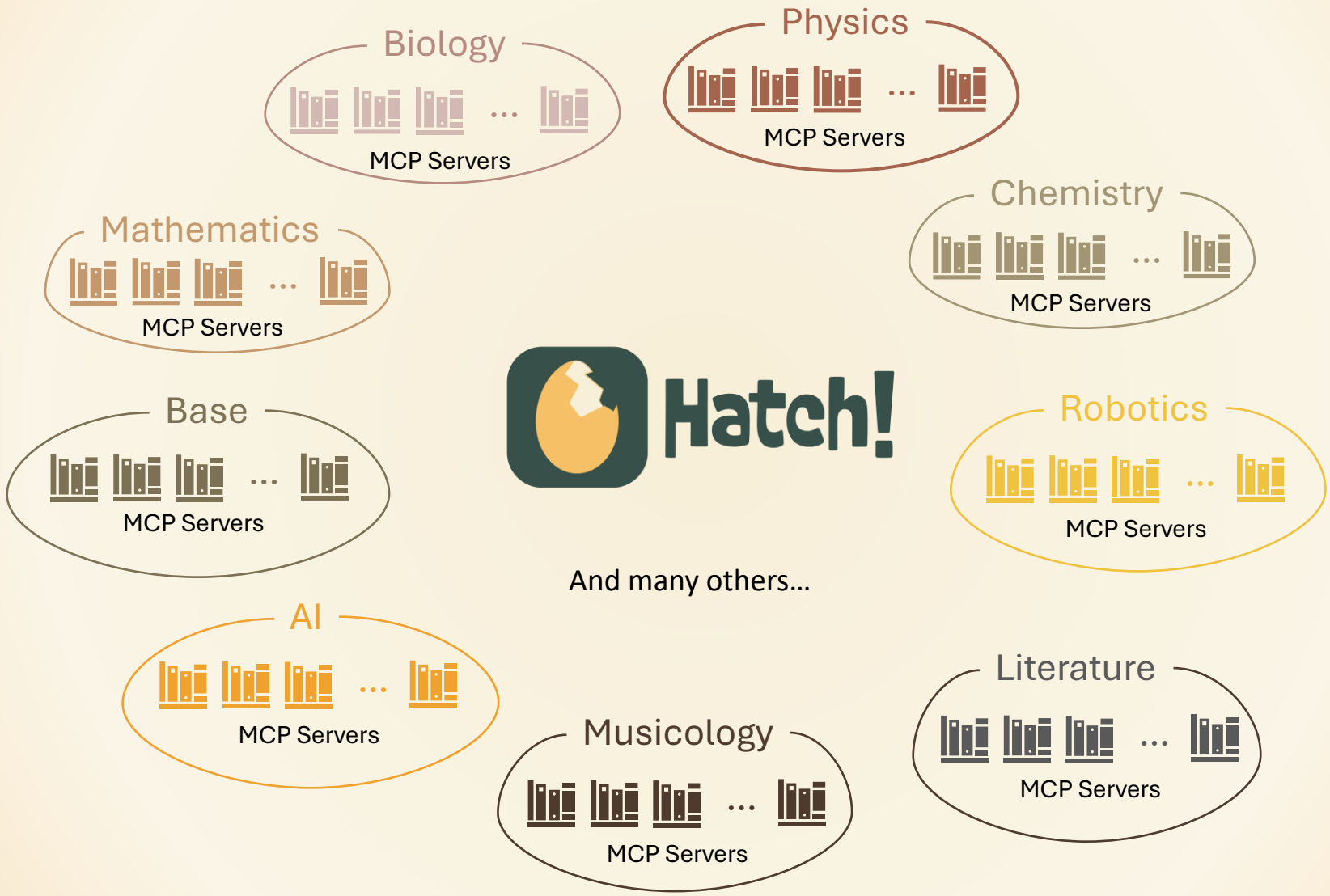
https://github.com/CrackingShells/Hatchling

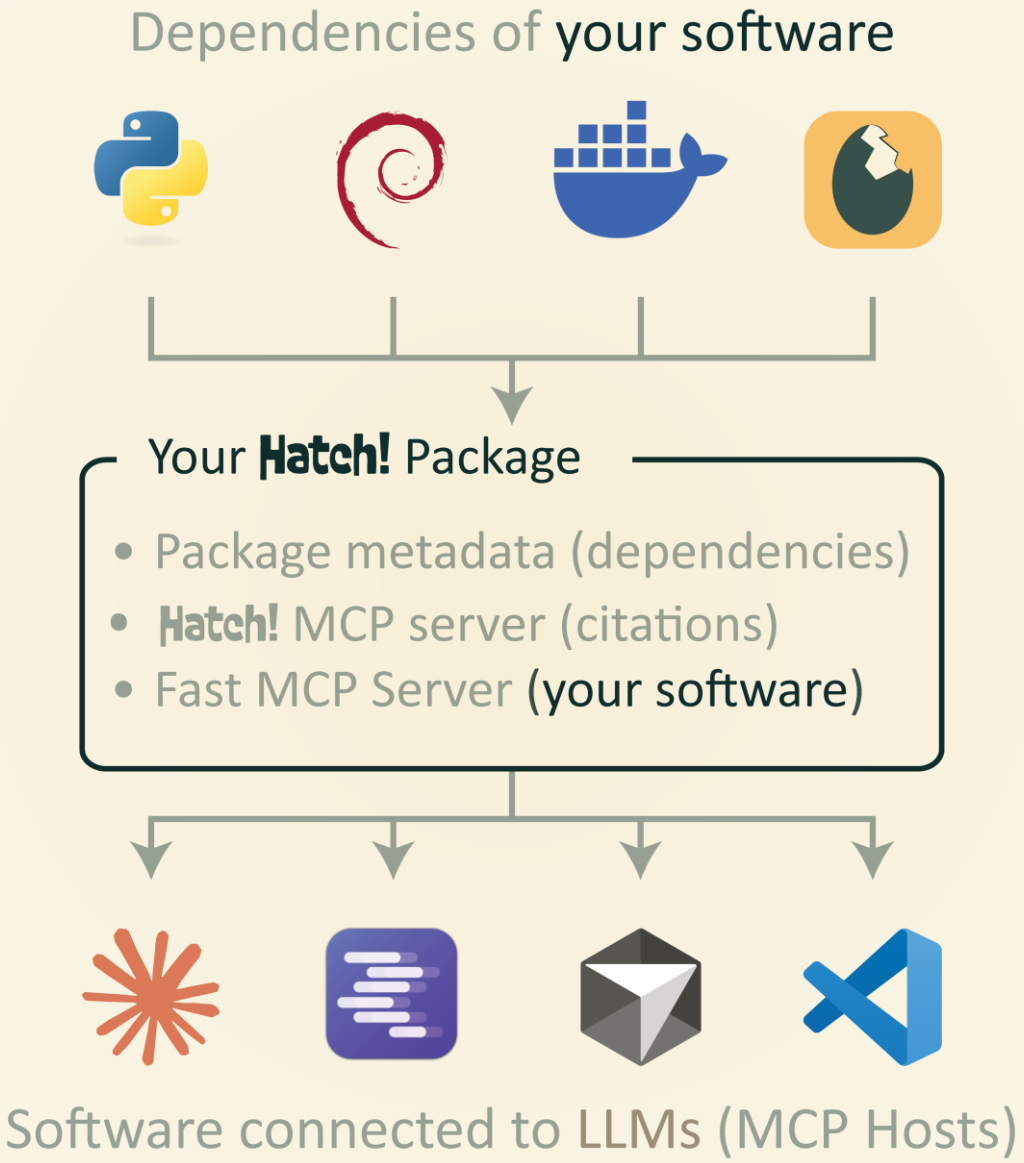
- **Hatch-Registry – The registry to gather Hatch packages**
- Hatch-MCP-Server – A wrapper around FastMCP to add a few things (**compatible with your vanilla MCP servers**)
- Hatch-Schemas – The schemas used for validating the packages and the registry’s structure
- Hatch-Validator – The logic to validate the packages and registry

Hatch! to install your servers



The vision


Biology
MCP Servers
Physics
MCP Servers
Chemistry
MCP Servers
Mathematics
MCP Servers
Hatch!
Base
MCP Servers
Robotics
MCP Servers
And many others...
AI
MCP Servers
Musicology
MCP Servers
Literature
MCP Servers


Dependencies of your software
Your Hatch! Package
• Package metadata (dependencies)
• Hatch! MCP server (citations)
• Fast MCP Server (your software)
Software connected to LLMs (MCP Hosts)

Configuring MCP servers in any MCP Hosts

In `v0.7.0.dev8`

GEMINI-CLI

```
hatch mcp configure <server_name> \
   --host <mcp_host_name> \

   --command <command> \
OR
   --url <url>
```

And many options…

Claude

Migrating MCP servers between MCP Hosts

In `v0.7.0.dev8`

GEMINI-CLI

```
hatch mcp sync \
    [--server <server_name>] \
    --from-host <host_name> \
    --to-host <coma-sep host_name>
```

Claude

A couple use case

Example: From modelling to simulation

Dr. Ruscone
@BSC

https://github.com/marcorusc/mcp-biomodelling-servers

Hatch!

User

"Prompt"

Hatchling

Host

Remote LLM

gpt-4o-mini
gpt-5

MCP server
NeKo

16 tools for network constructions

NEKO

https://sysbio-curie.github.io/Neko/

MCP server
PhysiCell

19 tools for 2D & 3D agent-based simulations

PhysiCell
powerful · extensible · cross platform

https://physicell.org/

MCP server
MaBoss

14 tools for boolean network simulations

MaBoSS

https://maboss.curie.fr/

Paper:
https://arxiv.org/abs/2508.18489