

How to Make Your Science Easier with AI Support

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Date: October 3rd, 2025

Time: 10:00–12:00

Location: I2SysBio Seminar Room

by our PhD student: **Tianyuan Liu**

October 3rd, 2025

Genomics 
 of Gene
Expression Lab

Outline

1. Introduction to AI-Assisted Development
2. Context Engineering
3. Responsible AI & Production Best Practices
4. Conclusion

Quick Poll: Your AI Experience

Let's see where everyone is!

1. Who uses LLMs?
(ChatGPT, Gemini, Claude for conversations)
2. Who uses coding agents?
(GitHub Copilot, Cursor, Claude Code, Gemini CLI)
3. Who uses agents for everything?
(Slides, CVs, research papers, full workflows)

Raise your hand for each one!

Quick Start: Quick Install

```
1 # Using npx (no installation required)
2 npx https://github.com/google-gemini/gemini-cli
3
4 # Install globally with npm
5 npm install -g @google/gemini-cli
6
7 # Install globally with Homebrew (macOS/Linux)
8 brew install gemini-cli
9
10 # Requirements: Node.js v20+, macOS/Linux/Windows
```

Workshop Structure

What We'll Cover

Live Demos

1. Introduction to AI-Assisted Development
ReAct, MCP, Tools
2. Context Engineering
Guiding AI effectively
3. Responsible AI & Production Best Practices
Best practices & quality
4. Conclusion
Future directions

- ▶ Demo 1: Research slides
LaTeX generation from papers
- ▶ Demo 2: CV generation
Context engineering in action
- ▶ Demo 3: React website
Unit testing & CI/CD

Hands-on + Theory for practical AI-assisted research

Let's Get Started: Clone the Repository Clone the Workshop Materials

```
1 git clone  
  https://github.com/TianYuan-Liu/ai-agent-workshop
```

This repository contains:

- ▶ All demo examples
- ▶ LaTeX templates
- ▶ Configuration files
- ▶ README with setup instructions

Please clone this now so you can follow along with the demos!

LLM vs. AI Agent

Large Language Model

- ▶ Cannot use tools

Example: ChatGPT (basic mode)

AI Agent

- ▶ Tools: Execute actions
- ▶ Memory: Context retention
- ▶ Planning: Multi-step tasks

Example: Cursor, Gemini CLI

$$\text{Agent} = \text{LLM} + \text{Tools} + \text{Memory} + \text{Planning}^{[1]}$$

Reason Only and Act Only



Reason Only



Act Only

ReAct (Reason + Act)

ReAct



(Reason + Act)^[2]

Why Do We Need MCP?

The Missing Link

ReAct combines reasoning and action, but lacks a standardized, reliable interface for taking actions.

Without MCP

- ▶ Custom code for each AI agent
- ▶ Tools stay invisible to AI

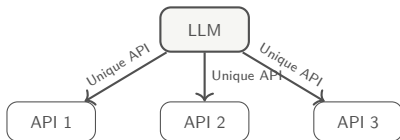
With MCP

- ▶ One protocol for all agents
- ▶ AI finds and uses tools itself

MCP = The bridge enabling ReAct to work in practice^[3]

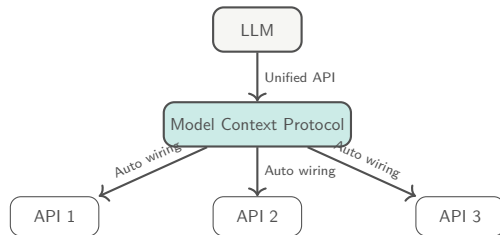
API vs MCP: Before and After

Before MCP



Traditional API
You write code

After MCP



MCP
AI uses tools

MCP = APIs that AIs can find and use by themselves

API vs. MCP: Concrete Example

Task: "What's the weather in Valencia?"

Using Traditional API

You must code:

```
1 import requests
2
3 def get_weather(city):
4     url = "https://api.weather.com"
5     params = {"city": city}
6     response = requests.get(url, params)
7     data = response.json()
8     return data["temp"]
9
10 # Call it manually
11 temp = get_weather("Valencia")
12 print(f"Temperature: {temp}C")
```

**Problem: You write & maintain all
integration code**

Using MCP

MCP Server provides:

```
1 {
2     "name": "get_weather",
3     "description": "Get current weather",
4     "parameters": {
5         "location": {
6             "type": "string",
7             "description": "City name"
8         }
9     }
10 }
```

AI automatically:

- ✓ Reads the schema
- ✓ Knows when to call it
- ✓ Passes correct parameters
- ✓ Interprets the response

MCP Call Flow: How It Works

Understanding Client-Server Architecture

The Players

Client: The AI agent

Server: Your MCP tool provider

Client asks, server does the work

The Call Flow

1. Client connects → `list_tools`
(gets tool schemas)
2. AI chooses tool + arguments
3. Client → `call_tool(name, args)`
4. Server runs code → returns data
(hits APIs, DB, shell, etc.)

Key: AI never sees your implementation, just the interface

Why MCP Is More Secure

Security Through Controlled Access

The Risk

Model has no direct power

Only calls tools you expose

But if model sends personal data:

- Client forwards it
- Server processes it
- Data could leak out

Warning: Privacy risk once data leaves

MCP Protection

1. Schema constraints

Strict field validation

2. Scoped servers

Only run what you trust

3. Local by default

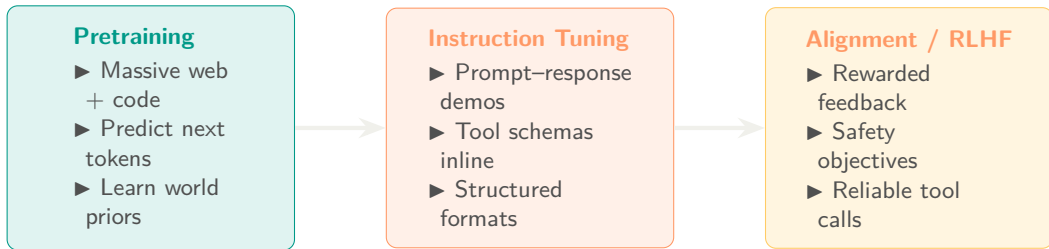
Data stays on your machine

4. Auditing/logging

Track all tool calls

Bottom line: You control what tools exist and where data flows

How LLMs Learn Tool Use^[4]



ReAct in Action: RNA-Seq Workflow

Task: “Deliver QC-ready RNA-seq counts for today’s batch.”

1. **Thought:** “Need QC thresholds before planning.”
2. **Action:** `read_file("GEMINI.md")`
3. **Observation:** “Standards: reads >10M, FRiP >0.2.”
4. **Thought:** “Plan pipeline using those gates.”
5. **Action:** `launch_rnaseq_qc(batch="2024-10-01", min_reads=1e7)`

Result: `counts.tsv` + `qc_report.html` ready for review.

Agent Stack for Scientific Workflows

Agent Ingredients

- ▶ Foundation model reasoning
- ▶ ReAct planning loop
- ▶ MCP tool catalog

Human Inputs

- ▶ GEMINI.md + project context
- ▶ Quality gates & constraints
- ▶ Review & acceptance criteria

Bridge: This stack powers the upcoming demos for slides, CVs, and production code.

Definition

ReAct loops for planning, writing, testing & refining code autonomously^[2].

Where They Shine

- ▶ Automate repetitive QC or plotting
- ▶ Scaffold pipelines & tests
- ▶ Keep research notes in sync

What You Still Own

- ▶ Set objectives & constraints
- ▶ Provide project context
- ▶ Review & sign off outputs

Next: Watch this collaboration build research slides.

Demo 1

Coding Agent for Research

Generating LaTeX Slides from Research Papers

Scenario: Journal Club Presentation

The Situation

It's 10 PM. You have a journal club presentation tomorrow morning at 9 AM.

- ✓ You've finished reading the paper
- ✗ You have **no time** to create slides
- ✗ You're exhausted and need sleep

Solution: Let an AI agent create the slides for you!

The agent can read the paper, extract key points, and generate a professional presentation while you rest.

Live Demo: Coding Agent for Research

Goal Turn the epigenome review into polished slides with a ReAct loop.

Setup

- ▶ Workspace: `examples/demo1/`
- ▶ Read `prompt.txt`
- ▶ Use Conesa theme

Loop

1. Think: ground in prompt + paper
2. Act: write slides, manage assets
3. Observe: compile, adjust

Checklist

Compile cleanly; figure rule respected; log key decisions.

What Is Context Engineering?

Key Insight^[5]

“Most agent failures are context failures, not model failures.” — Tobi Lütke, Shopify

Core Components

Instructions
Project Context
Domain Knowledge
Examples

Context = Better AI

Specificity beats vagueness
Examples beat explanations
Constraints beat preferences

Guiding AI for Multi-Omics Analysis

Simple Strategy

Tell AI your **data type** + **quality rules** + **ask for a plan**

RNA-seq Example

```
QC RNA-seq FASTQs, align to  
GRCh38, generate counts.
```

```
Quality: $>$10M reads
```

```
Output: counts.tsv
```

ATAC-seq Example

```
Process ATAC reads, call peaks  
with MACS2.
```

```
Quality: FRiP $>$ 0.2
```

```
Output: filtered_peaks.bed
```

Key: Specific data type + QC thresholds + reference to GEMINI.md

Anatomy of a Research GEMINI.md

```
1 # Project: Multi-omics Data Analysis
2
3 ## Data (CRITICAL)
4 - IRB: #2024-456 | Data: RNA-seq, ATAC-seq
5
6 ## Tech
7 - STAR (GRCh38), MACS2, RGmatch, Python 3.11
8
9 ## Domain
10 - RNA-seq QC:  $>10M$  reads | ATAC-seq QC: FRiP  $>0.2$ 
11
12 ## Stats
13 - Correlation networks for omics integration | FDR: BH | Seed:
    42
```

Key Sections: Privacy • Tech • Domain • Stats

Context Engineering Best Practices

DON'T

“Write good code”

12 pages of docs

Outdated specs

DO

Functions < 50 lines

Core concepts only

Living document

Remember: Examples > Explanations

Demo 2

Context Engineering in Action

Building a LaTeX CV from Web Forms

Scenario: Academic CV Maintenance

The Challenge

You need a professional CV for job applications. Updating it is tedious.

The Pain Points:

- × Manually adding new publications, talks, awards
- × Maintaining LaTeX formatting consistency
- × Different formats for different positions

What info should you give an AI agent to automate this?

Demo 2: Context Engineering for LaTeX CV Generation

The Workflow

Web form → Structured prompt → AI creates CV

Your Task

1. Open `examples/demo2/index.html`
2. Fill in the form

Key Insight

Form shows what AI needs:

- ▶ Personal details
- ▶ Education & experience
- ▶ Skills & projects

What Is Vibe Coding?

Definition^[6]

“A new coding style where you embrace exponentials and forget the code even exists.”
— Andrej Karpathy

Vibe Coding

Prompt → Generate → Run

No Review!

Responsible AI

Prompt → Generate → REVIEW

Test → Deploy

The Research Integrity Framework

Code Type	Examples	AI Usage
Exploration	Visualizations, Conversions	✓ Vibe OK
Production	Pipelines, Tools	AI + Review
Critical	Statistics, Publications	× Traditional

Real Risks for Researchers

Security^[7]

- ▶ 40% of AI code has flaws
- ▶ Prompt injection
- ▶ Hardcoded credentials

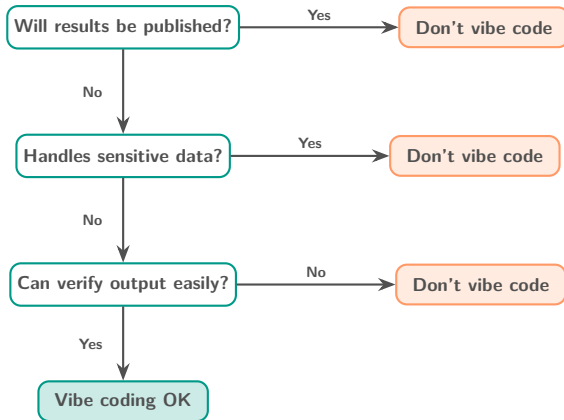
Reproducibility

- ▶ Non-deterministic
- ▶ Can't verify
- ▶ Journals need disclosure

Surprising Finding^[8]

- ▶ Experienced devs: 19% slower with AI on complex tasks

Best Practices Decision Tree



Keeping Vibe Coding in Check

1. Ask for a step-by-step plan before work starts

Example: “Make a step-by-step plan for RNA-seq QC analysis”

Agent outputs: 1. FastQC on FASTQs 2. MultiQC reports 3. Flag <10M reads 4. Summary stats

2. Review and approve the plan before execution

✓ Review agent’s proposed steps and approve or modify

3. Have the agent make a to-do list to track progress

Track completion: ✓ Done ▶ In progress Pending

Why GitHub Matters

AI agents iterate fast, mistakes happen — **version control is critical** for tracking, rollback, and collaboration.

Key Benefits

- ▶ Track every change
- ▶ Easy rollback
- ▶ Safe collaboration

Workflow

1. Branch → Generate
2. Review → Commit
3. Pull request → Merge

What is CI/CD?

Auto-test and deploy AI code on every commit.

Unit Tests

- ▶ Fast feedback
 - ▶ Catch regressions
- pytest, Jest, JUnit

CI/CD Flow

1. Push code
2. Auto-test & lint
3. Block if failing
4. Deploy if passing

GitHub Actions

Demo 3

Production-Ready AI Code

React Website with Unit Testing & CI/CD

Scenario: From Development to Production

The Challenge

AI agents build bioinformatics tools fast. But how do you deploy them **safely** to production?

- ? How to catch bugs before users do?
- ? How to ensure reliability with new data?
- ? What are the best practices?

Answer: Unit testing + CI/CD pipelines

Demo 3: Unit Testing & CI/CD in Practice

Building a React CV Website with Automated Testing

What's Tested

- ▶ Component rendering
- ▶ Data validation
- ▶ User interactions
- ▶ Accessibility (a11y)

`npm test` — runs all tests

CI/CD Workflow

1. Push to GitHub
2. Tests run automatically
3. Lint & format check
4. Build production site
5. Deploy to GitHub Pages

Location: `examples/demo3/` — See `README.md` for full guide

Next Step: Fully Autonomous Agents

Why This Matters

The next evolution of AI agents is full computer control so they can execute end-to-end workflows without human clicks.

- ▶ **Example:** Agent-TARS plans and books trips autonomously.
- ▶ **Capability:** Interfaces with web apps, files, and APIs to manage travel logistics while you supervise outcomes.
- ▶ **See it:** <https://agent-tars.com/>

Takeaway: Prepare workflows and safeguards so agents can operate safely when they get full desktop control.

The Last Agent?

Embodied Intelligence brings AI into the physical world.

- ▶ **Unitree G1:** Anti-gravity mode trained via reinforcement learning. Watch: https://www.youtube.com/watch?v=bPSLMX_V38E
- ▶ **Figure AI:** Humanoid robot that can do your dishes autonomously. Watch: <https://www.youtube.com/watch?v=8gfuUzDn4Q8>

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- [3] Anthropic. *Introducing the Model Context Protocol*. Anthropic Blog. Technical documentation for Model Context Protocol. Nov. 2024. URL: <https://www.anthropic.com/news/model-context-protocol>.
- [4] Yujia Qin et al. “Tool Learning with Foundation Models”. In: *arXiv preprint arXiv:2304.08354* (2023). Survey on how foundation models learn to use external tools. URL: <https://arxiv.org/abs/2304.08354>.

References II

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- [6] Andrej Karpathy. *Vibe Coding: A New Paradigm in AI-Assisted Development*. Personal Blog. Accessed: 2025-10-01. Feb. 2025. URL: <https://karpathy.ai/>.
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