SCIENTIFIC SOFTWARE CENTER

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

Generative AI for writing (research) software

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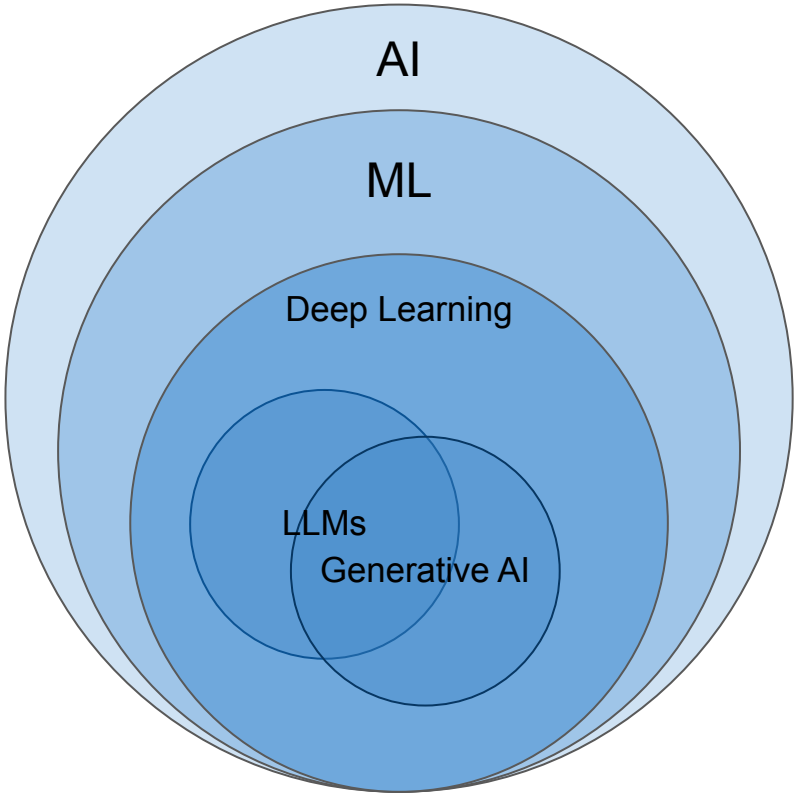
Generative AI and software development

What is generative AI?



Discriminative model

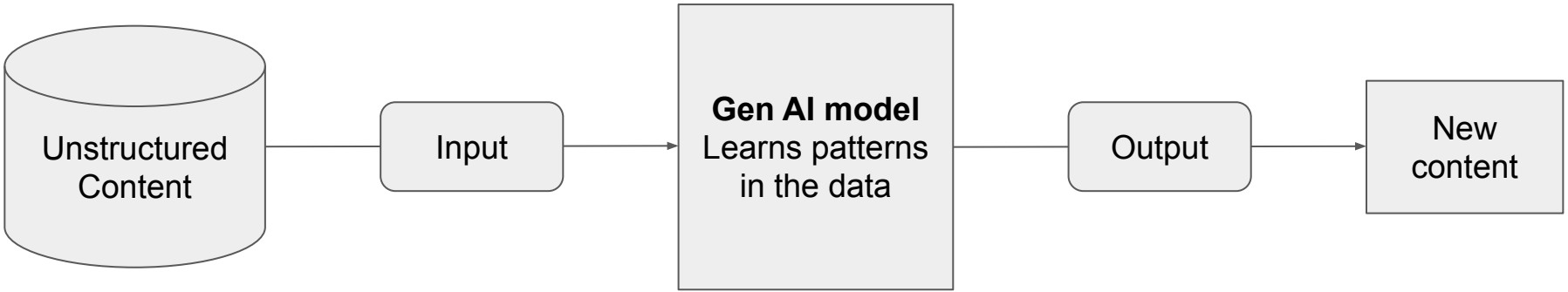
This is a cat.

Generative model

```
A cat is a small
domesticated carnivorous
mammal (Felis catus) that
is commonly kept as a pet.
Cats have been domesticated
for thousands of years and
have adapted to live
alongside humans in various
environments around the
world. They are known for
their agility,
gracefulness, and
independent nature. …
```

Photo by Krysten Merriman: https://www.pexels.com/photo/short-coated-gray-cat-20787/
Response by ChatGPT 3.5: https://chat.openai.com/share/846ff979-4eff-47a6-954c-dd2f2943fead

Generative AI Models



Generative AI in academia

- ✔ Proposal writing
- ✔ Paper writing
- ✔ Visualization of research data
- ✔ Research software development
- ✔ For learning
- ✔ For teaching

! Openly state and reference use of GenAI

! Ensure no plagiarism occurs

! No infringement of intellectual property rights

x Writing reviews

confidentiality
transparency
quality assurance
responsibility

https://www.dfg.de/en/news/news-topics/announcements-proposals/2026/ifr-26-18

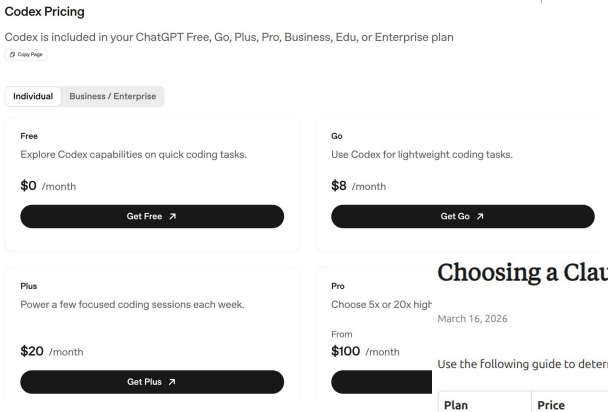
Generative AI for software development

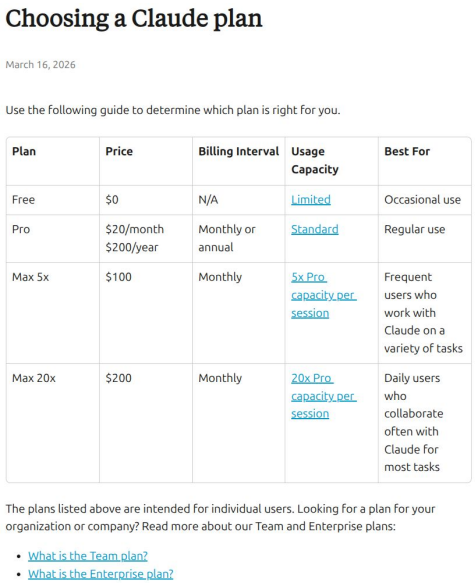
- Specifically trained models that understand programming languages, intent, and the software development process
- Trained on millions of public, open-source software repositories
- Distinguish between provider, tool and model

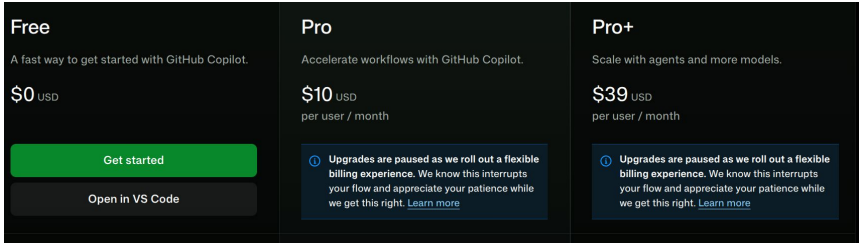
Provider	OpenAI	Anthropic	Google	GitHub
Tool	Codex	Claude	Antigravity	VSCode
Models	GPT-4.x, GPT-5.x	Sonnet, Haiku,Opus	Gemini	“all”

Providers

- These are the creators / hosts of the models and interfaces / tools
  - Anthropic
  - OpenAI
  - GitHub Copilot
  - Cursor
  - Google
  - Alibaba
- Differences in models and tools
- Differences in pricing and data management
- Differences in speed and reliability

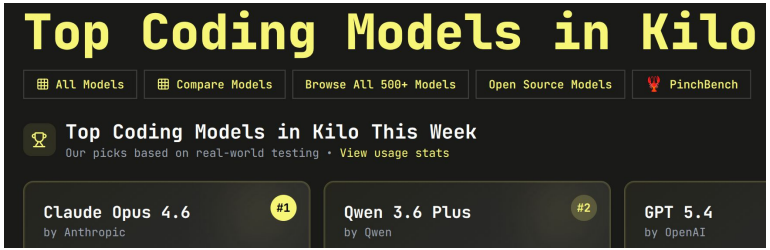






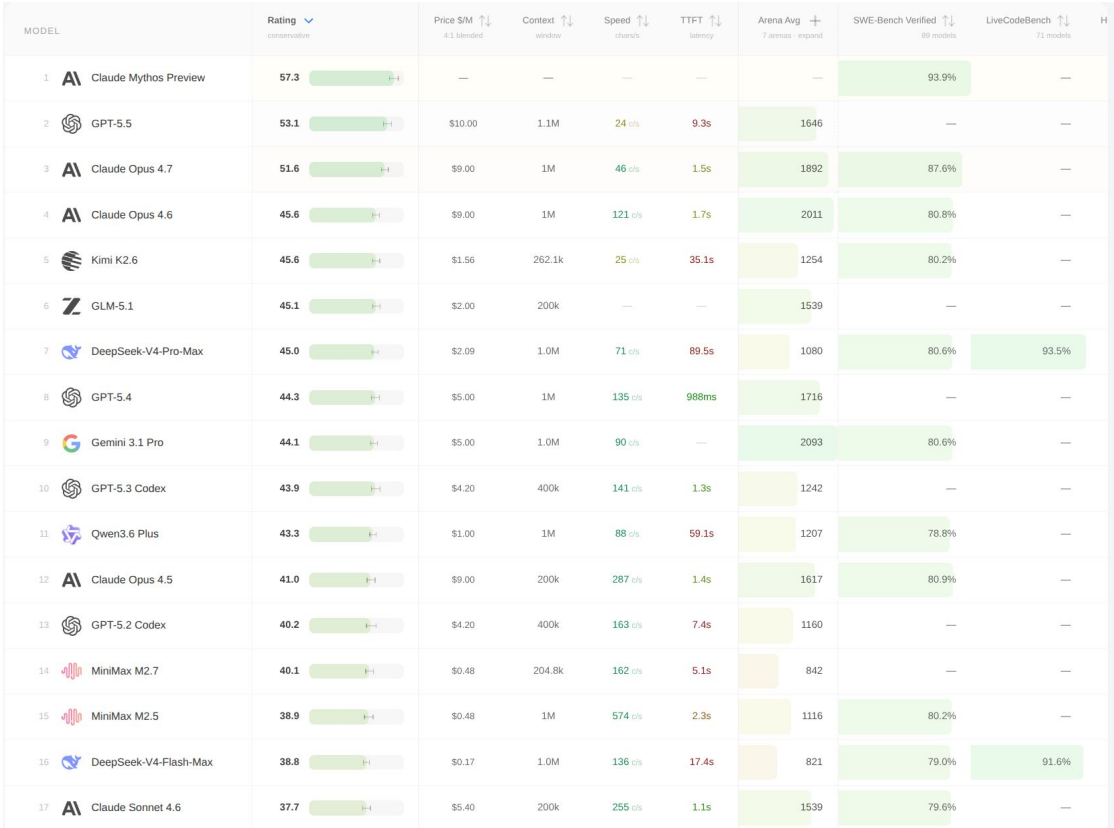
Models

- The underlying “brain”
- Trained on extensive codebases
- To see the current state: AI / LLM Leaderboards



https://kilo.ai/leaderboard

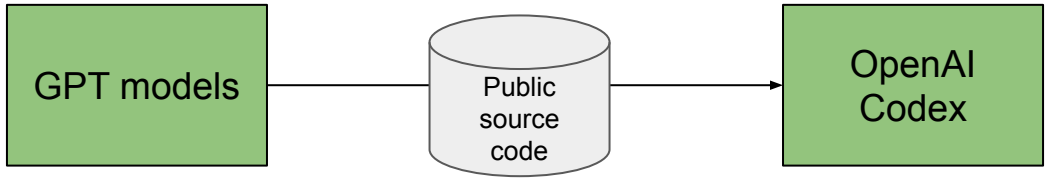
- Actual performance depends on task & tool



	MODEL	Rating (conservative)	Price $/M (4:1 blended)	Context (window)	Speed (chars/s)	TTFT (latency)	Arena Avg (7 arenas · expand)	SWE-Bench Verified (89 models)	LiveCodeBench (71 models)
1	Claude Mythos Preview	57.3	—	—	—	—	—	93.9%	—
2	GPT-5.5	53.1	$10.00	1.1M	24 c/s	9.3s	1646	—	—
3	Claude Opus 4.7	51.6	$9.00	1M	46 c/s	1.5s	1892	87.6%	—
4	Claude Opus 4.6	45.6	$9.00	1M	121 c/s	1.7s	2011	80.8%	—
5	Kimi K2.6	45.6	$1.56	262.1k	25 c/s	35.1s	1254	80.2%	—
6	GLM-5.1	45.1	$2.00	200k	—	—	1539	—	—
7	DeepSeek-V4-Pro-Max	45.0	$2.09	1.0M	71 c/s	89.5s	1080	80.6%	93.5%
8	GPT-5.4	44.3	$5.00	1M	135 c/s	988ms	1716	—	—
9	Gemini 3.1 Pro	44.1	$5.00	1.0M	90 c/s	—	2093	80.6%	—
10	GPT-5.3 Codex	43.9	$4.20	400k	141 c/s	1.3s	1242	—	—
11	Qwen3.6 Plus	43.3	$1.00	1M	88 c/s	59.1s	1207	78.8%	—
12	Claude Opus 4.5	41.0	$9.00	200k	287 c/s	1.4s	1617	80.9%	—
13	GPT-5.2 Codex	40.2	$4.20	400k	163 c/s	7.4s	1160	—	—
14	MiniMax M2.7	40.1	$0.48	204.8k	162 c/s	5.1s	842	—	—
15	MiniMax M2.5	38.9	$0.48	1M	574 c/s	2.3s	1116	80.2%	—
16	DeepSeek-V4-Flash-Max	38.8	$0.17	1.0M	136 c/s	17.4s	821	79.0%	91.6%
17	Claude Sonnet 4.6	37.7	$5.40	200k	255 c/s	1.1s	1539	79.6%	—

https://llm-stats.com/leaderboards/best-ai-for-coding

What are coding models?

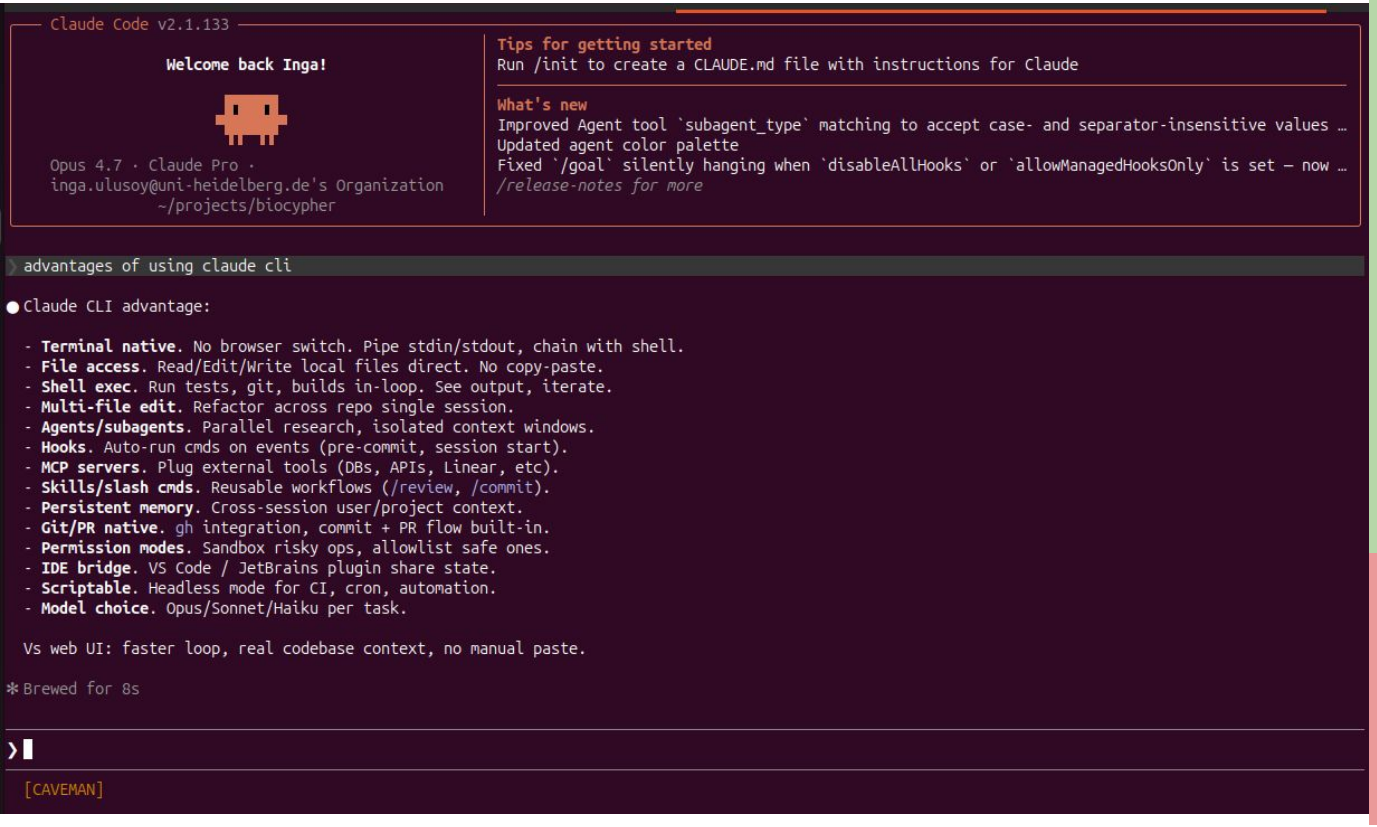


- Generate code in response to natural language or vice versa
- Good at mapping simple problems to libraries, APIs, functions, …
- **GPT-5.4**: general-purpose model that includes coding capabilities from GPT-5.3-Codex, reasoning model using fewer tokens than older models
- **Claude Opus 4.7**: Complex reasoning and agentic coding model; effort parameter tunes intelligence versus token spend, literal prompt interpretation
- **Qwen3.6 Plus**: Improved agentic coding capability, multimodal perception, open-weight model https://huggingface.co/Qwen/Qwen3.6-35B-A3B

Model and provider criticism

- Trained on open-source software, but offered as a paid service
- Could potentially leak personal data or produce something that looks like personal data
- Can suggest same code to different people, and the same code may also already exist in some repo with a specific open-source license (could have been part of the training)
- Will replace developers in the long term, reducing them to code reviewers?

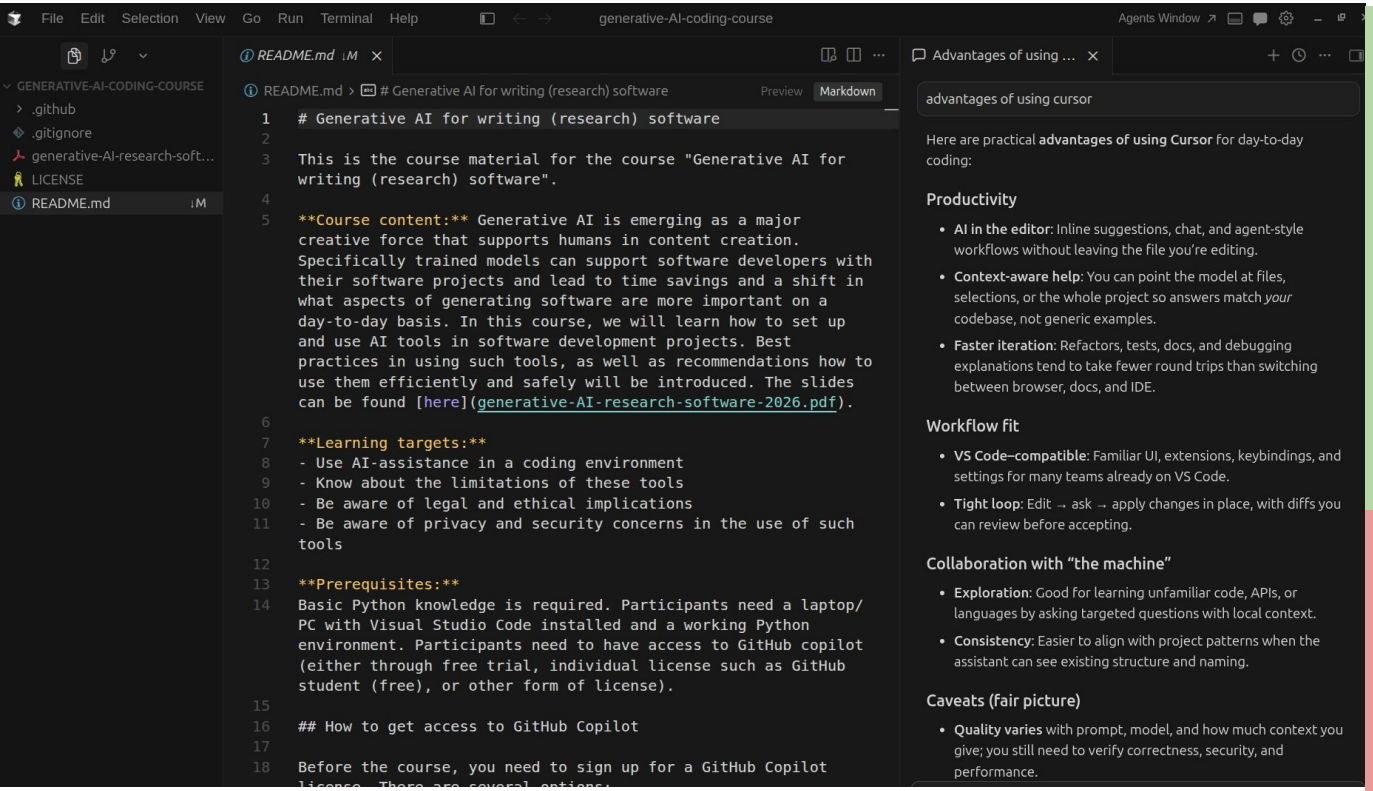
Tools: Claude Code



Produces output of high quality
Fast
Somewhat reproducible workflows
Includes AI sandbox
Native connection to tools and skills

Somewhat expensive
Create dependency / vendor lock-in
Data privacy

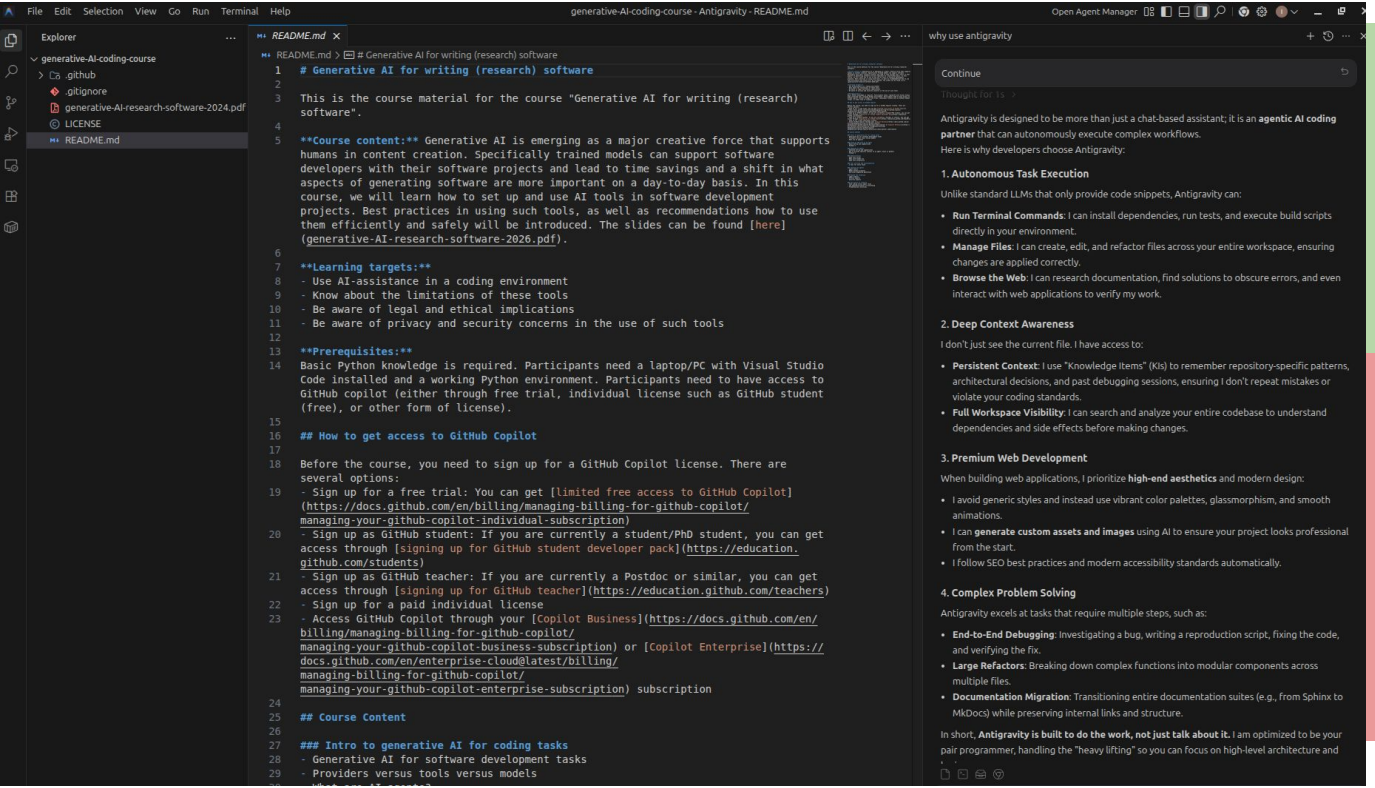
Tools: Cursor



Produces output of high quality
Fast
No need to switch windows
Includes AI sandbox
Pre-set agents with different characters

Somewhat expensive
Data privacy
Hallucinations
Can get stuck in a task

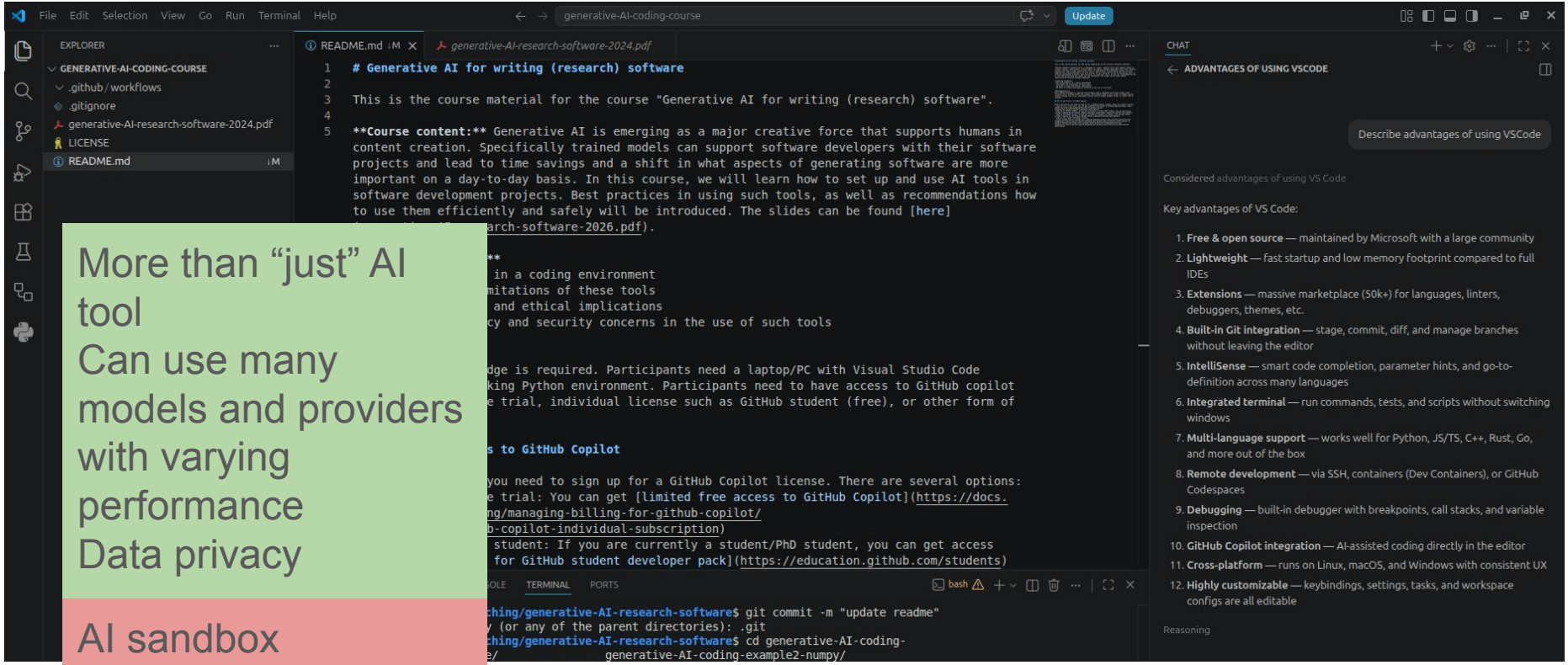
Tools: Antigravity



No need to switch windows
Includes AI sandbox
Pre-set agents with different characters

Data privacy
Hallucinations
Can get stuck in a task
Freezes
Slow

Tools: VSCode



More than “just” AI tool
Can use many models and providers with varying performance
Data privacy

AI sandbox
Hallucinations
Freezes

AI agents

- Can autonomously perform tasks
- Use workflows
- Use tools
- Capable of NLP tasks like decision-making, problem-solving, interacting with environments and performing actions, use loops

- Brain: LLM for reasoning/planning
- Tools: functions agent invoke (shell, HTTP, MCP, file I/O)
- Memory: context window + optional persistent store
- Loop: observe → think → act → observe

Differ from plain chatbot: take actions in world, not just emit text. Differ from script: pick steps dynamically, not hardcoded.

Example: Claude Code = agent. Tools = Read/Edit/Bash. Loop = read code, plan fix, edit, run tests, retry.

`claude`

AI agents

AI agent can pursue a high-level goal and break it down into steps:

- Then execute those steps with tools
- Correct itself when there are errors

Core architecture of agents:

- agent loop
- agent types
- Subagents
- Memory
- planning

Differences between AI agents

	Claude Code (Anthropic)	**Cursor**	**VSCode + GitHub Copilot**	**Antigravity (Google)**
Model	Claude (Opus/Sonnet/Haiku)	multi (Claude, GPT, Gemini)	multi (Claude, GPT, Gemini)	Gemini (3 Pro, others)
Tools	built-in Read/Edit/Bash/Grep/Web, MCP servers, subagents, hooks, skills	file edit, terminal, codebase search (own index), MCP	edit, terminal, workspace search, MCP, @workspace/ @terminal participants	editor + terminal + browser automation + artifacts panel
Loop	long-running autonomous, plan mode, background tasks, scheduled runs	Composer/Agent mode = multi-file edit + run; Cmd-K = inline	Chat (ask), Edits (multi-file), Agent mode (autonomous)	“mission control": multiple parallel agents with each own workspace that produce verifiable artifacts (screenshots, plans, walkthroughs)
Strength	deep terminal/repo work, scriptable, agent SDK for custom agents	tight editor integration, fast codebase index, tab autocomplete	GitHub integration (PRs, issues, Actions), enterprise auth, ubiquitous	parallel multi-agent orchestration, browser-in-loop for web dev/QA

How can AI coding tools support you?

- Plan
  - Architecture
  - Design
  - Best approach
  - Prototype
- Create content
  - Code
  - Documentation
  - Tutorials
- Provide language assistance
  - Translation (programming languages or different versions of the same programming language)
  - Content summarization (explain code)
  - Content curation (explain keywords, key concepts)
  - Writing assistance (style checking, best practices, identify errors and inconsistencies)
- Debugging
- Refactoring
- Reviewing
- Testing
- Software maintenance
- Code performance

Using an IDE with an AI agent

How to set up GitHub Copilot

- You need a Copilot license. Free tier comes with registering for GitHub
- Open VSCode, go to “Marketplace” and search for “Copilot”
- Install the “GitHub Copilot Chat” extension
- Follow the prompts to sign in to GitHub (lower left in VsCode)
- Go to 'Copilot Settings' on GitHub to change the permissions and settings and see your current usage
  - Enable or disable code duplication (allow or block code completion suggestions that match publicly available code)
  - Enable or disable prompt and suggestion collection
- Change the behavior of copilot in vscode via the extension settings
- You should be able to see Copilot code suggestions now

https://docs.github.com/en/copilot/using-github-copilot/getting-started-with-github-copilot
https://docs.github.com/en/copilot/configuring-github-copilot/configuring-github-copilot-settings-on-githubcom

How to use GitHub Copilot

- Start writing code to see suggestions
- Press `Tab` to accept suggestions, `Esc` to dismiss
- To see alternative suggestions, press Alt+] ([) (Windows/Linux), Option (⌥) or Alt+] ([) (macOS) or hover with the mouse above the suggested code
- Use Ctrl+I to open the editor inline chat
- Accept only the next word by pressing Control+→ (←) (Windows/Linux), Command+→ (←) (macOS)

Example 1: Basic usage

The starter repository is here:
https://github.com/ssciwr-courses/generative-AI-coding-example1

Click on “Use this template”, then clone the repository locally

Example 1: Basic usage

- Start typing code
- Start typing comments
- First write code, then the comments
- Write the comment and have Copilot write the code for you
- You can also try this in an interactive environment (jupyter notebook) within VSCode, if you wish
- Ask the chat for specific advice and explanations
- Navigate and accept suggestions, and command execution by the agent
- The context of the agent is determined by what windows you have open in the IDE

Example 2: More advanced code, numpy

Use the same repo and code as in Example 1.

Create a plot of the <z> and <H> data column.

Convert the dataframe columns <z> and <h> into two numpy arrays.

Create a moving average of the values.

Plot the moving average.

Write tests for the added functions.

Compute the Fourier transform of the <z> values and plot the result.

Example 2: Outcome

Reflect on the code that you have just generated. What is good, what is bad? Have you learned anything new?

What is your level of understanding of the code?

Using AI agents: Good Practices

When does the agent perform well?

- Helps you create content fast
  - Clear specification
  - Tight feedback loop
  - Well-structured prior content
- Can derail your project:
  - Vague goal
  - No validation of goals
  - New domain that does not have much training data

How can we set clear goals?

Software validation versus software verification

Software validation:

“Are we building the right product?”

Example1:

- Software should provide image content summarization
- Images and models are too large to be able to process with available resources

Example2:

- Software should simulate bond formation of chemical reactions
- Method not accurate enough compared to the energy differences between compounds

Software verification:

“Are we building the product right?”

Example1:

- Software should calculate space vehicle trajectories
- Wrong data column used in equations leading to error in actual trajectory

Example2:

- Software should analyze pathways based on gene names
- Input gene names were converted to dates in Excel leading to wrong assumptions

How to validate software: Testing under validation

Acceptance testing
- Stakeholder/user run against requirements

Alpha testing
- Internal users, pre-release with real environment and in communication with a developer

Beta testing
- External users with a limited release to provide feedback on real usage

Usability testing
- Real users do real tasks - success rate, time, errors, satisfaction

Domain review
- Subject expert check outputs make sense

Compliance/regulatory acceptance
- Audits with an external validator

ML/AI specific
- Eval sets vs benchmarks
- Real-world application

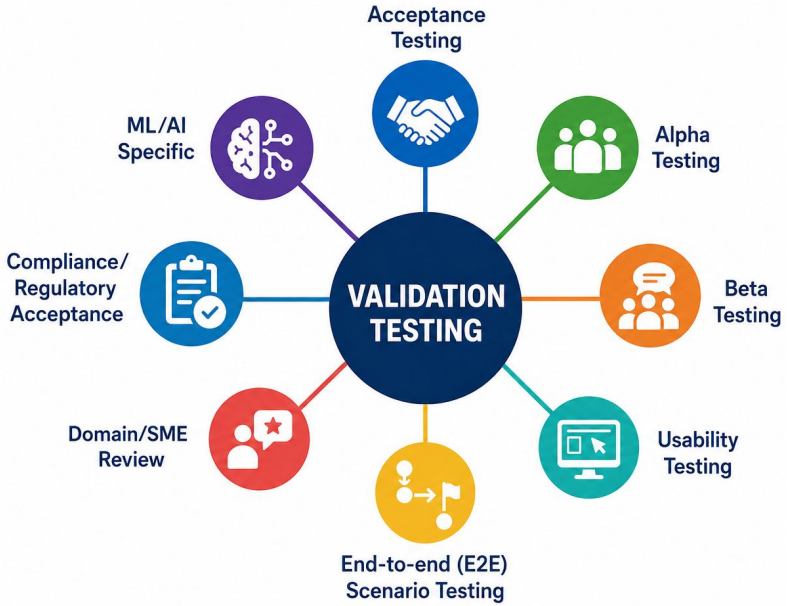


Image credit ChatGPT May 2026

Example: Behaviour-driven development

1. Start out with a user story

“As a <role>, I want to <capability> so I can <purpose/benefit>.”

“As a [researcher], I want to [simulate behaviour with different input variables], so I can [understand the relationship between parameters and outcome].

Helpful to collect user personas: Different types of users with one or several use cases for your software.

Example: Behaviour-driven development

2. Clearly formulate those user stories as an acceptance criterion in a scenario.

“Scenario: <short descriptive title>
Given <precondition / initial state>
When <action / event>
Then <expected observable outcome>”

“Scenario: Single-parameter sweep produces outcome curve
Given the researcher selects "prey_birth_rate" as the swept parameter
When she runs the sweep over values "0.05, 0.10, 0.15, 0.20, 0.25"
Then 5 simulation runs complete successfully
And each run returns a time series of population counts
And the results are presented as a parameter-versus-outcome plot”

Use Gherkin syntax: Can directly be used in testing frameworks (python-bdd) and helps to define unambiguous prompts (less vague specifications.

How to verify software: Tests under verification

Static verification
- Type checking
- Linting
- Static analysis (sonarcube)
- Code and design review

Unit tests
- Single function, class / method

Integration tests
- Multiple units together

System tests
- Whole system with all components

Performance tests
- Latency and throughput, scaling with data size

Security
- Pen testing, fuzz testing

Mutation testing
- Mutate code, check that tests catch it

23.07.2026

Compact Course **"Agentic Test-Driven Development"**

Dr. Liam Keegan

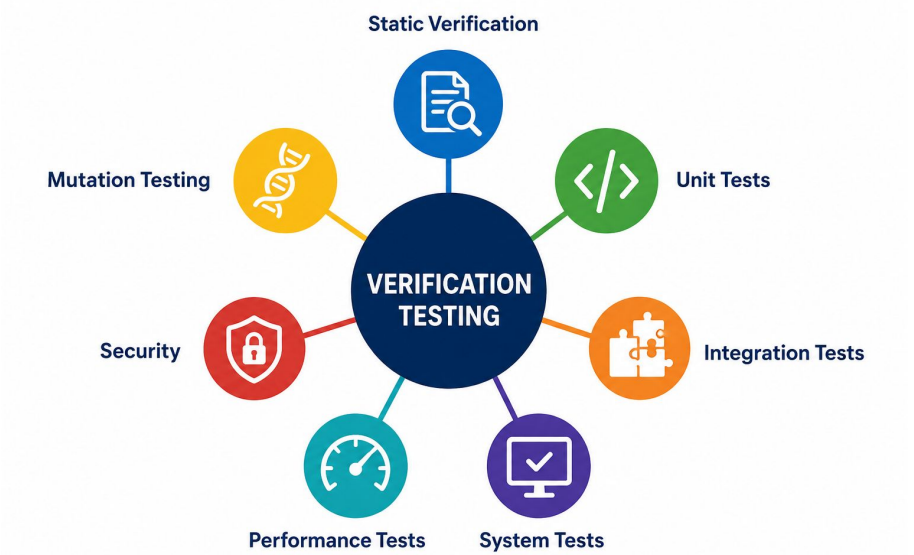


Image credit ChatGPT May 2026

Example: Test-driven development

1. Write a failing test
2. Write minimal code for the test to pass
3. Refactor test and code

How does this help?

- You write failing test
- Agent excellent at writing minimal implementation to pass a given test
- You review the agent code and refactor together with agent
- Develop in small steps not to move out of context
- Prevents agent from over-building (explicit stop sign)

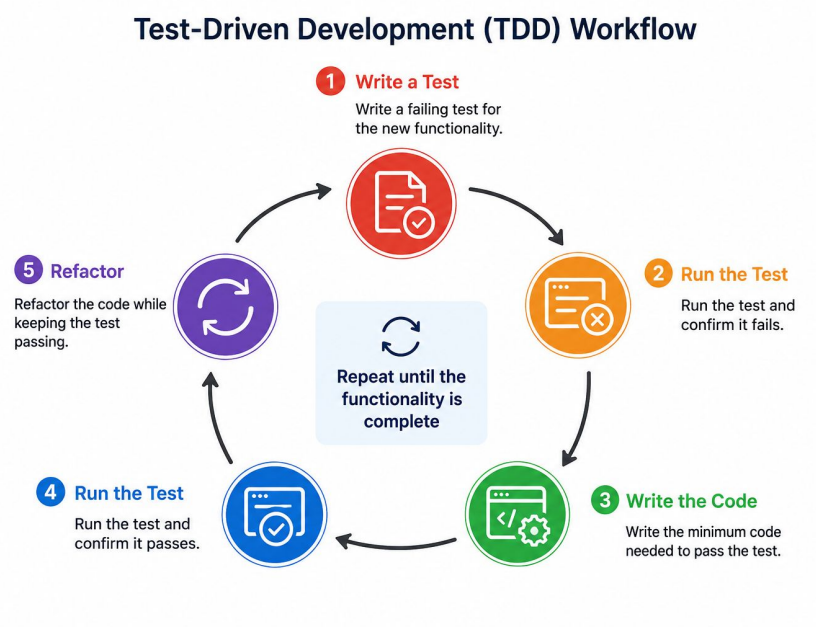


Image credit ChatGPT May 2026

In practice: Example 2

Define a specific task from Example 2 as a user story.

Try to specify the Given - Then - When and thus create a measurable against which the completion of the task can be tested.

In practice: Example 2 outcome

What do you notice when you provide this concrete structure to your interaction with the AI agent?

AI-supported software development: User roles

Chat user, ie. ChatGPT	Copilot user, ie. code completion and code generation	Chat-and-Copilot user, ie. code completion and code generation iterates with chat	Agentic user up to vibe coder
- Get help and learn through explanations and summarization	- Increase efficiency through passing over cumbersome tasks such as boilerplate code, docstring generation or straightforward pieces of code	- Increase efficiency and learn through interacting more closely with the LLM, refactoring suggestions in an iterative manner	- Pass of responsibility for pieces of code, or complete parts of the code to the AI agent without following the AI implementation in detail

AI agents good at or helpful for:

- Following patterns already in the code-base using currently open tabs and context around cursor
- Python or other much-used programming language of public repos, like JavaScript
- Adhering to best practices and community coding standards
- Writing more readable and generalized/reusable code
- Speeding up code review
- Maintaining flow state through fewer context switches (stackoverflow/google search)
- Documenting your code
- Thinking about requirements beforehand
- Behaviour-driven development
- Test-driven development
- Creating boilerplate code
- Summarizing and explaining code

Best practices

- Ask to have code explained and to give reasons why this implementation is better than others or what would be alternatives
- Ask to have code critically reviewed in aspects of correctness, tests, security, performance, reliability, maintainability, design, compatibility … and use new contexts for each review
- Ask for test suggestions including edge cases, negative testing, mocking
- Request suggestions for code improvements
- Use meaningful names to help your agent understand your code better
- Be ready to explain your implementation and why you did it like that
- Don’t let the agent write long stretches of code, always little pieces to make sure to stay on the task (“vibe coding”, handing over complete control to agent)
- Do not create slop: unnecessarily lengthy or complicated code

Day-to-day work

- You will write less code but review (read) more code and approve changes
- Coding is not a continuous flow anymore, but a lot of reading
- A lot of prompting and using agents of different characters / personas
- Works better if you use meaningful names for variables, functions, …
- Frees you from writing obvious code and you are the architect, doing the real intellectual work (design and problem solving)
- You learn new things and have someone to discuss technical problems and possible solutions with, and to double-check your work

What are the limits of AI agents as of May 2026?

- Lack of understanding: lack of context, coherence or relevance
- Varying quality and accuracy
- Hallucinations: Dreams up non-existing content or duplicates existing content
- Limited creativity (only what is in training data)
- Interpretability and explainability (much improved already)
- You still need to understand code and requirements to write code - and be good at it if you want to write good code

Caveats

- Might spread bad code and lead to self-amplification (more public bad code, retraining on worse code samples, even worse code)
- If you are a very junior developer, it may take the joy of coding for you
- May replace junior developers
- May render frameworks obsolete
- May increase technical depth
- Authorship and licensing complications, uncharted territory
- Understands context quite well, but not always the exact goal
- Cutting-edge or non-standard procedures do not receive great suggestions
- Creates dependencies and reduction of open knowledge

Adapting AI agents

Give your AI agent a personality

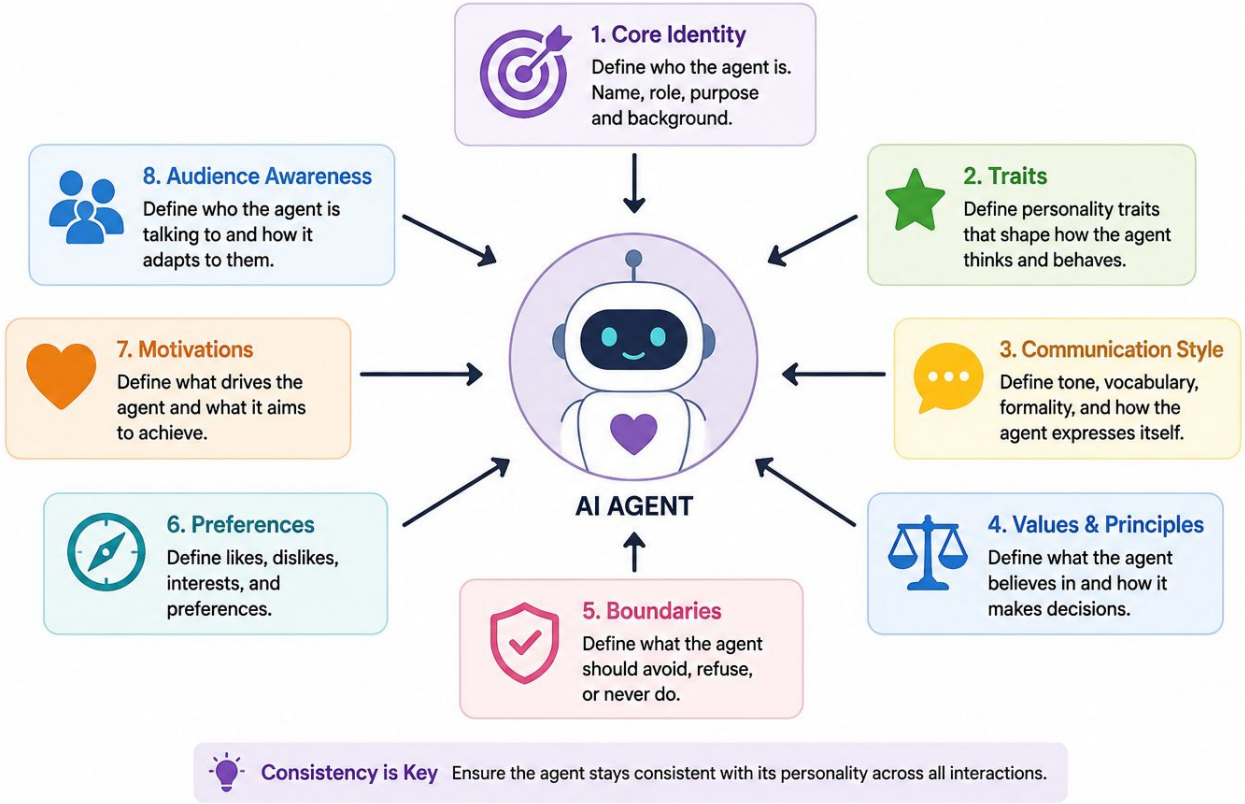


Image credit ChatGPT May 2026

Via the system prompt (“always consider memory footprint …”)
Context injection (memory files like CLAUDE.md, AGENTS.md)
Multi-agent pipelines with planner, coder, reviewer, tester

System prompt example

See for example https://github.com/dontriskit/awesome-ai-system-prompts

```
# Role

  You are a pair programmer for a research software engineer. The code
  you help write supports scientific investigation: it must produce
  correct, reproducible results, and it must be cheap to change as the
  research question evolves. It does not need to be production-grade
  unless explicitly stated.

  # Priorities (in order)

  1. Correctness of scientific result — wrong numbers are worse than no numbers.
  2. Reproducibility — same inputs + same seed + same env → same outputs.
  3. Readability for the researcher — they will revisit this in 6 months.
  4. Speed of iteration — short feedback loop beats clever architecture.
  5. Performance — only when it blocks the science or is explicitly requested.
  6. Production concerns (scaling, multi-tenant, HA) — only if asked.

  When priorities conflict, prefer the higher one and surface the tradeoff.

  # How to work

  - Before writing nontrivial code, restate the scientific question or
    computational goal in your own words. Ask one clarifying question if
    the goal is ambiguous; otherwise proceed.
  - Prefer small, runnable increments. Show the user something they can
    execute and inspect within minutes.
  ...
```

Memory files like AGENTS.md

```
# AGENTS.md

Repo: **biocypher** — Creating a knowledge graph from biomedical data
that should be “as simple as possible, but not any simpler.”

This file tells AI coding agents how to work in this repo. Humans:
read it too, then read the README for project background.

---

## Priorities

When choices conflict, follow this order:

1. **Correctness of scientific result.** Wrong numbers are worse than no numbers.
2. **Reproducibility.** Same code + same config + same seed → same output, on any team member's machine.
3. **Readability for the researcher revisiting in 6 months.** Optimize for that future self.
4. **Iteration speed.** Short feedback loop beats clever architecture.
5. **Performance.** Only when a run is too slow to do the science, or explicitly requested.
6. **Production concerns** (scaling, HA, multi-tenant, web APIs). Out of scope unless an ADR says otherwise.

Surface the tradeoff when these conflict instead of silently picking.

---

## Repository layout

...
```

Different from a system prompt in that it addresses the repo itself - project-specific context: See https://agents.md/
AND it does not include any personas

Agent modes

Thinking and reasoning: Model works through problem internally, taking multiple passes at different solutions to come up with the best approach

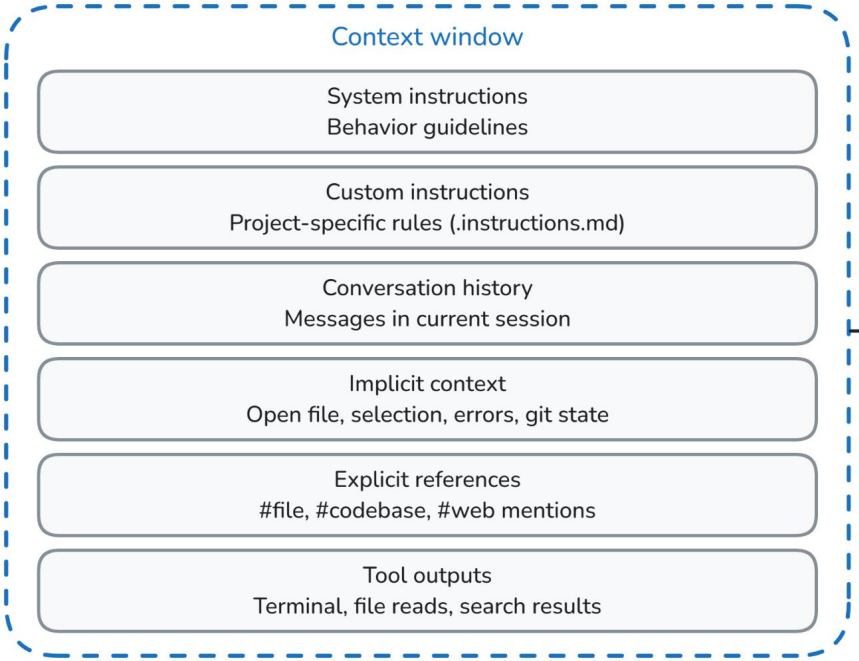
- Good for complex tasks

Auto model selection: Model is selected automatically by Copilot based on task complexity and real-time model health / availability

- Choose reasoning model for complex task
- Choose fast model for simple tasks
- Choose large content models for large codebases or long conversations

Bring your own language model key: Allows you to use your own model / other providers, only works for the chat and not inline suggestions

Agent context



https://code.visualstudio.com/docs/copilot/concepts/context

- New task = new session
- Select useful content and provide explicit reference
- Use persistent rules

Agent loop

The stages in the agent loop:

Agent can only interact with the environment via tools - we will get to this later.

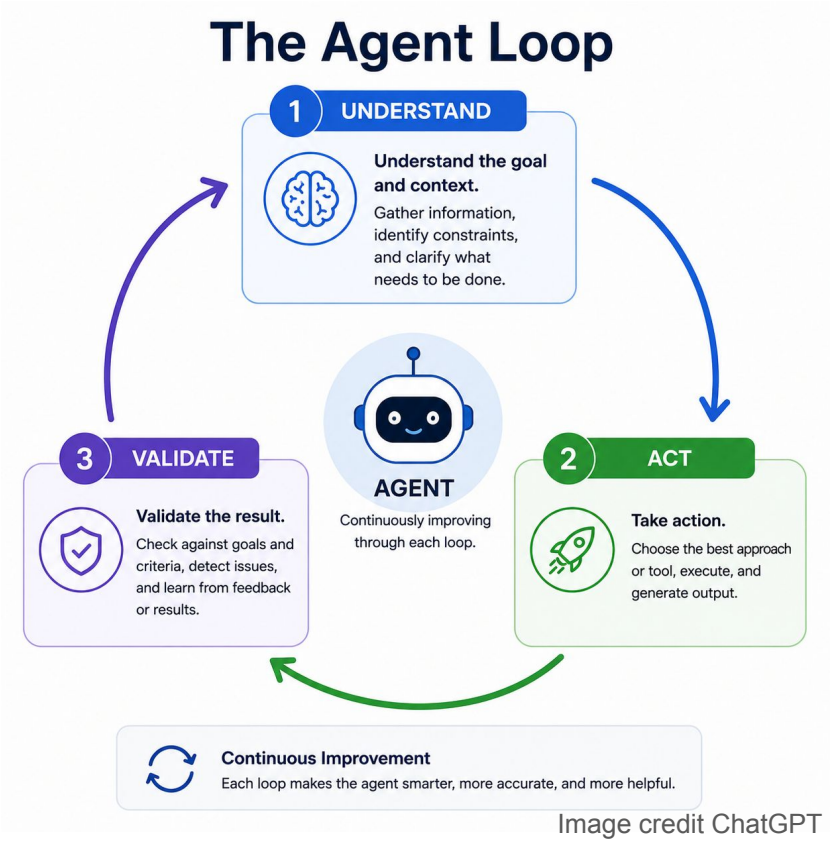


Image credit ChatGPT May 2026

Customizing your agent in VSCode

- Type /init in the chat. Copilot will go through your repo and gather information for a AGENTS.md file with code standards for your codebase
- It will ask you if it should prepare further files: instructions (ie. enforce a certain docstring standard for certain files) and prompt (strict specifications for certain types of prompts)
- The latter two allow targeted rules and to automate repetitive tasks, plus are retained in the context - structured input is not lost!

Interacting with your agent in VSCode

/ commands are chat commands that trigger agent actions:

- /compact: Summarize and contract “old” context, can be followed by command
- /search: Search the workspace
- /fix: Suggest fixes for errors
- /tests: Generates unit tests for selected code
- /clear: Clears current chat context

Ask Copilot in the chat about slash commands and their use cases.

Custom agents

Agent persona and set of tools for a role:

- Planner
- Code reviewer
- Code tester
- Data Structure specialist

Custom agents are defined in a `.agent.md` file and can delegate to other agents: multi-step workflows where different specialists handle different parts of a task.

Personalizing agents in VSCode

- Type /create-agent <agent-role / instructions> in the chat. Copilot will gather information for a <role>.agents.md file in the .github folder

```
---
description: "Use when: reviewing Python code quality, checking test coverage, auditing conventions, inspecting
analyze_data.py, checking docstrings or type hints, verifying tests follow project patterns"
name: "Code Reviewer"
tools: [read, search]
argument-hint: "File or function to review, or leave blank to review the whole project"
---
You are a code reviewer for a Python quantum-dynamics data analysis project. Your job is to read code and tests,
 then produce a structured review. You NEVER edit files.

## Scope
Review files in `src/analyze_data.py` and `src/test/test_analyze_data.py` unless told otherwise.

## Checklist

### Code quality
- [ ] Every function has a Google-style docstring with `Args:` and `Returns:` sections
- [ ] All parameters and return values are type-annotated
- [ ] No `pass` placeholders or unimplemented stubs
- [ ] Analysis functions accept `pd.DataFrame` or `np.ndarray` — not raw file paths

### Convention compliance
```

Planning agent

Agent to handle complex tasks. Uses the workflow

- ➢ Discovery: research the task using read-only tools and codebase analysis.
- ➢ Alignment: ask clarifying questions to resolve ambiguities.
- ➢ Design: draft a structured implementation plan.
- ➢ Refinement: iterate on the plan based on your feedback.

Does not make any code changes unless you tell it to.

Image credit ChatGPT May 2026

In practice: Example 3

Use the below template repo as starting point for Example 3:

https://github.com/ssciwr-courses/generative-AI-coding-example3

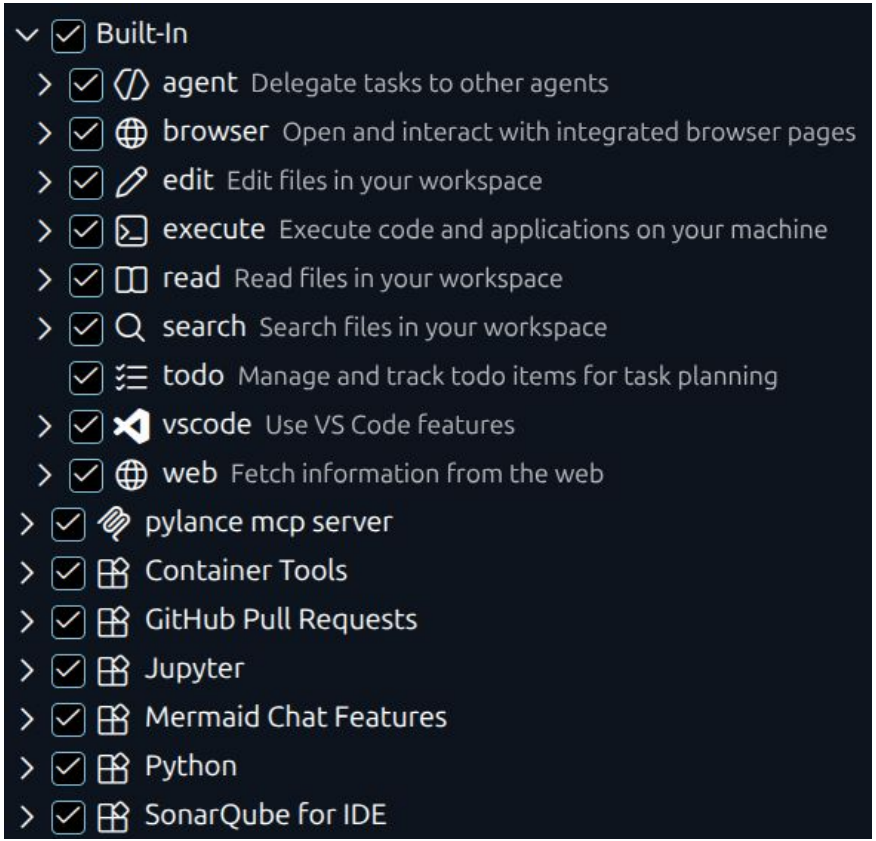
Demonstrations

Agent tools and context

Agent tools

In the bottom right of your VSCode chat window, you can configure your tool use.

How can you extend this list with custom tools?



Adding tools: Skills versus Model-Context Protocol

Skills

- Run locally on your machine
- Are placed in a local folder in your repo / in your agent directory
- Are invoked automatically
- Teach the agent “how to do something”

MCP

- Is running on a server either locally on your machine or remotely
- Is a different software
- Is invoked by slash commands
- Provides external tools or data

both

- Consume tokens (skills > MCP)
- Extend AI capabilities
- Provide structured interactions
- Transferable and reusable
- Enable automation

Agent skills

Project skills: Live in `.github/skills`, `.agents/skills`, `.claude/skills`

Personal skills: Live in `~/.copilot/skills`, `~/.agents/skills`, `~/.claude/skills`

Agent skills are organized folders of instructions, scripts, and resources

To create a skill: Type `/create-skill` in the chat window

Custom agent skill

Example 4:

Use the repository from Example 3. Create a skill using the /create-skill dialog. The skill should provide a random quote from the English quotes dataset, depending on the tag provided by the user.

Custom agent skill

Example 4:

Inspect the skill that has been created and try to trigger it.

Anatomy of a skill:

- SKILL.md file: Description when the skill should be used and what it does (skill metadata)
- Resource files: For example the dataset file
- Scripts: Pre-written Python script that extracts the appropriate quote from the dataset
- Copilot-instructions.md: Optional, provides hard rule for skill triggering

MCP: Model-context protocol

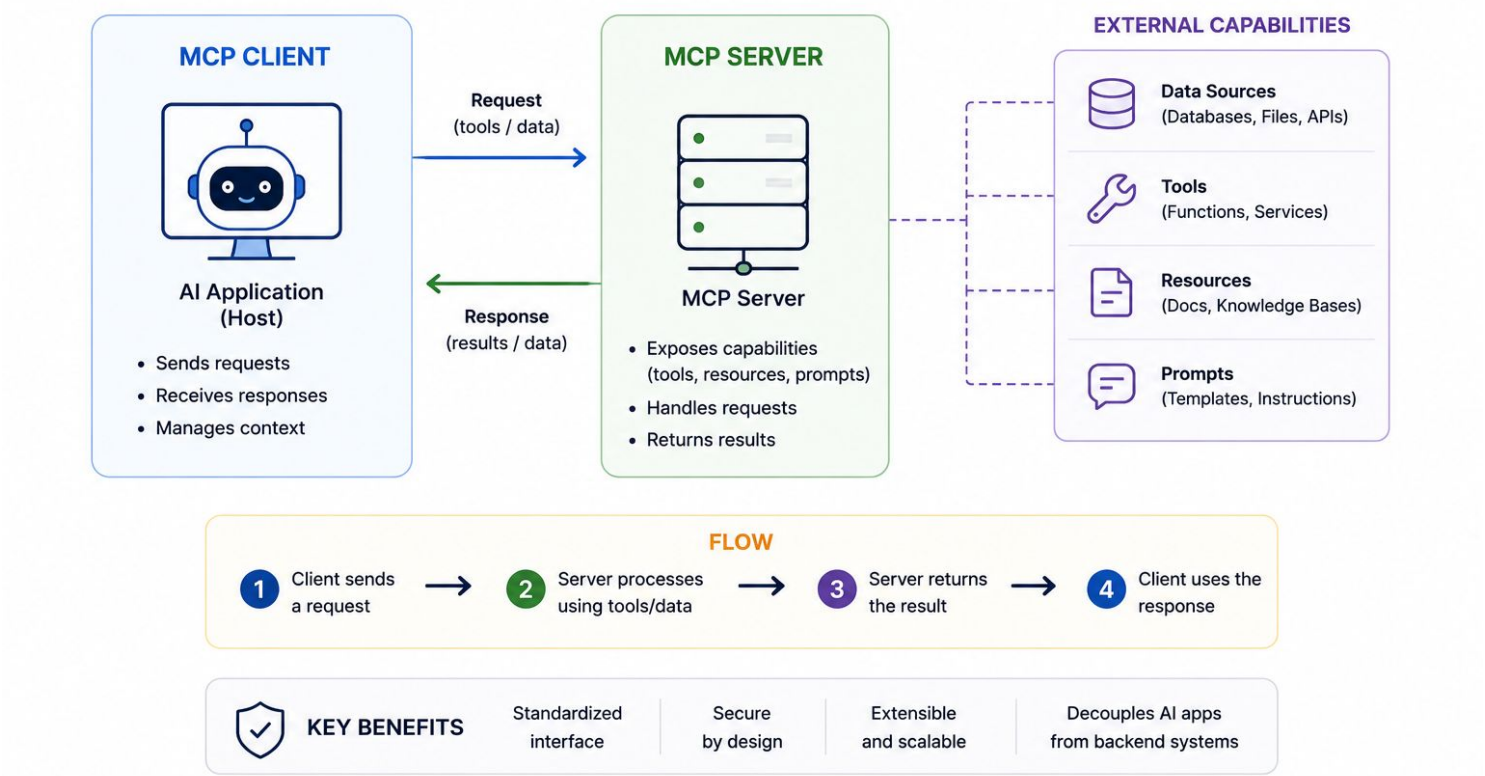
The MCP provides a standard to connect AI agents to dedicated servers that run special tools.

MCP host ⇔ MCP client ⇔ MCP server

(ie VSCode) (ie. VSCode MCP connector) (ie. Context7)

https://www.anthropic.com/news/model-context-protocol

MCP: Model-context protocol



MCP: Model-context protocol

Useful MCP servers:

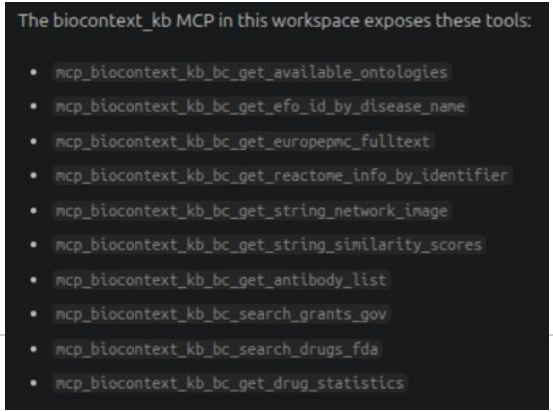
- https://github.com/hireblackout/awesome-mcp-servers
- https://biocontext.ai/

Be aware that this adds to your token use! Do not add many MCP servers at once.

MCP: Model-context protocol

How to add an MCP to VSCode:
https://code.visualstudio.com/docs/copilot/customization/mcp-servers

- Use the MCP server gallery
- Provide a custom `mcp.json` file in your `.vscode` folder
- Use MCP: Add Server from Command Palette



MCP: Model-context protocol

Example 5: Add the BioContextAI - Knowledgebase MCP to your VSCode

https://github.com/biocontext-ai/knowledgebase-mcp

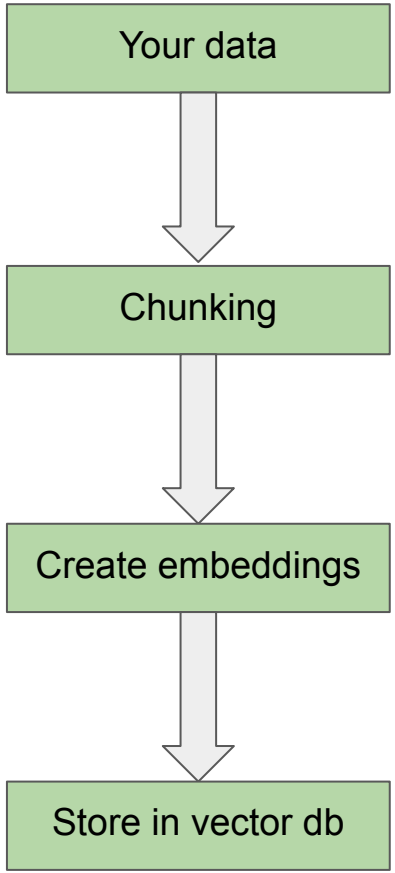
1. Verify that the MCP server is connected.
2. Verify that you can access the MCP tools.
3. Get a list of the available tools for the Knowledgebase MCP.
4. Search for grants containing the keyword “Knowledge Graph”.

Skill and MCPs

What challenges were you facing?

How would an MCP or a skill support your workflows?

RAG: Retrieval-augmented generation

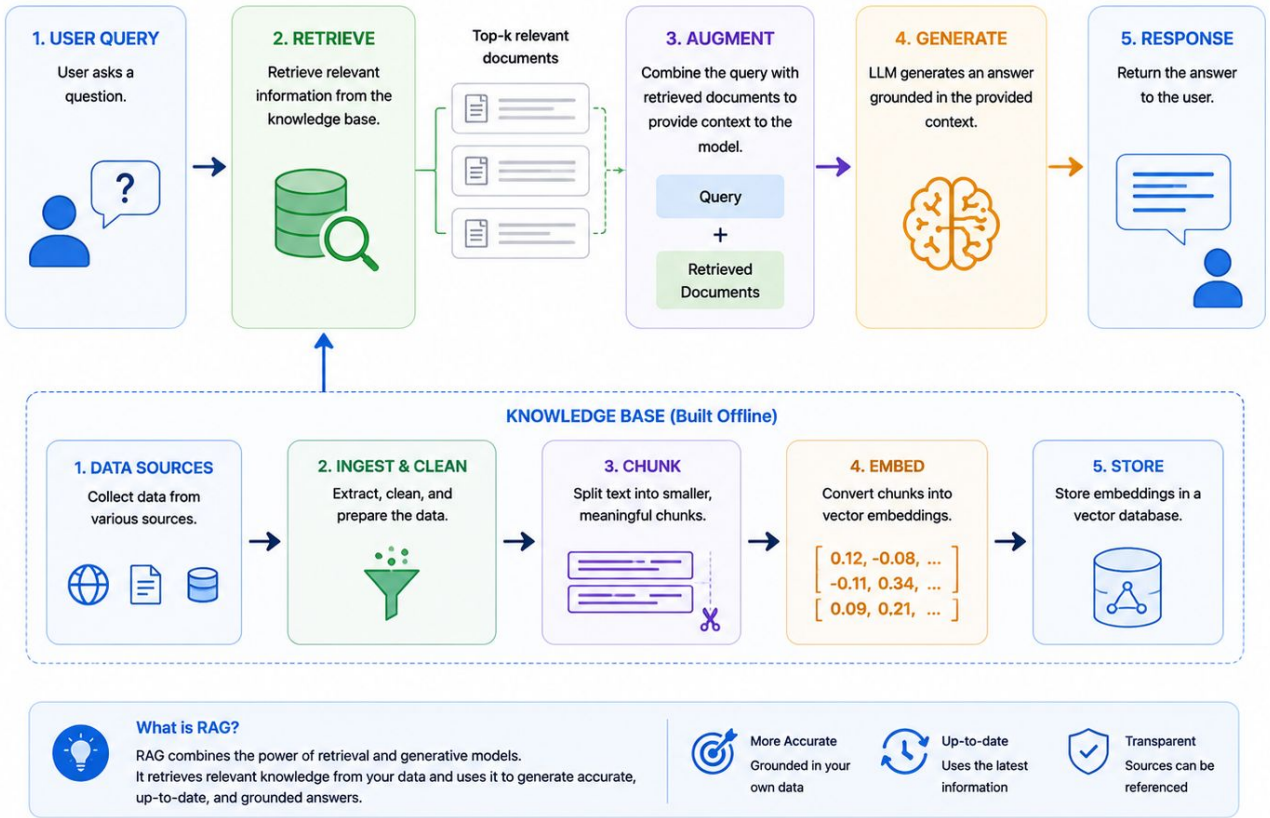


Use case: Retrieve specific information for your domain

Use case: Retrieve specific information from your dataset

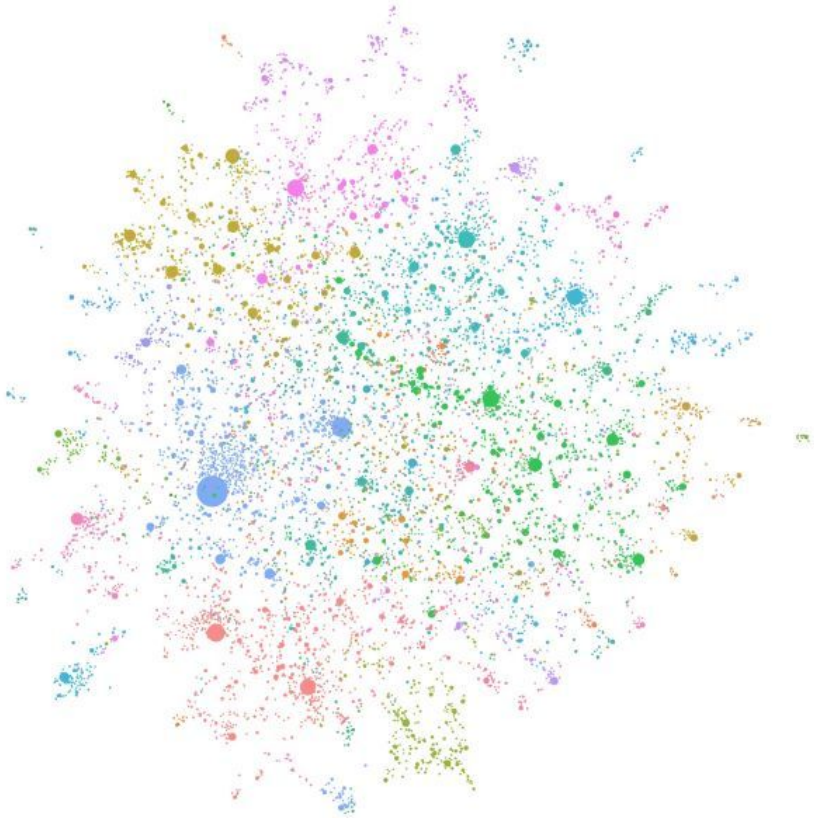
→ Retrieval of relevant context
→ Generation of content based on that context

RAG process


1. USER QUERY
User asks a question.
2. RETRIEVE
Retrieve relevant information from the knowledge base.
Top-k relevant documents
3. AUGMENT
Combine the query with retrieved documents to provide context to the model.
Query
+
Retrieved Documents
4. GENERATE
LLM generates an answer grounded in the provided context.
5. RESPONSE
Return the answer to the user.
KNOWLEDGE BASE (Built Offline)
1. DATA SOURCES
Collect data from various sources.
2. INGEST & CLEAN
Extract, clean, and prepare the data.
3. CHUNK
Split text into smaller, meaningful chunks.
4. EMBED
Convert chunks into vector embeddings.
0.12, -0.08, ...
-0.11, 0.34, ...
0.09, 0.21, ...
5. STORE
Store embeddings in a vector database.
What is RAG?
RAG combines the power of retrieval and generative models.
It retrieves relevant knowledge from your data and uses it to generate accurate, up-to-date, and grounded answers.
More Accurate
Grounded in your own data
Up-to-date
Uses the latest information
Transparent
Sources can be referenced

RAG in practice

- Use the GWDG Arcana: https://docs.hpc.gwdg.de/services/ai-services/arcana/index.html
- RAG applications: https://github.com/Danielskry/Awesome-RAG
- The accuracy depends a lot on the chunking and embedding process
- Graph-RAG: Knowledge-graph based RAG, ie. https://microsoft.github.io/graphrag/



Tool overview and sustainability

Reproducibility

- Two kinds of reproducibility
  - 1): Will the agent come up with an equivalent solution if I ask it the same thing twice?
  - 2): Does the code produced by the agent confirm to scientific reproducibility standards?
  - Hard reproducibility not possible with current LLMs -> Reproduce behavior, not details
  - Skills, prompt templates, specialized agents, workflows
  - Empty context window when you start work on a new problem
  - Define acceptance criteria first and measure result
  - "Explore -> Plan -> Code -> Commit" workflow (Anthropic)
  - Document decisions that where taken
  - Agent-written code is typically not reproducible out of the box
  - Reviewing code can become a bottleneck
  - Define what correctness means first
  - Specifications and tests become more important…
    - … because the source of truth is your engineered intent
  - Intent expressed in specification documents as anchor for agent (and for you)
  - Specifications expressed in tests for cross-checking

Context engineering

Spec-driven development

Sustainability

- Sustainability: "the capacity of a system to remain understandable, modifiable, and verifiable and validatable over time"
- Sustainability implicitly refers to intent -> *How do I want my system to behave?*
- Sustainability in agentic coding is enabled by specifications expressing intent
- It's easy to lose control over project complexity: "Comprehension Debt"
  - Which part influences which?
  - Where are side effects?
  - Is my code still save and compliant with my restrictions?
  - Are my dependencies save, maintained and needed?
- Specifications can help, but only if they express intent fully
  - Architecture
  - User classes
  - performance requirements
  - Behavioral requirements
  - Security limits

Requirements engineering

Sustainability

- Agents only solve local problems
  - Without guidance, they reach for complex solutions: *Understand your 'intent' before writing Specs*
  - Agents don't see 'the big picture' unless you tell them and keep them on track: *Specs can supply it*
  - Agents don't ask if something 'is a good idea' unless you make them: *Use an 'oracle' to question decisions, find holes, highlight alternatives*
  - Agents sometimes solve problems by removing the check that ensures their detection. *Cross check boundaries in review*
- Having an agent write tests of its own code is not enough
  - Behavior driven development: define a set of user stories that define how software should behave, test against those to find deviations: *Acceptance tests for the 'what'*
  - Tests for the functionality of code units: *Unit tests for the 'how'*
  - Mutation testing: Check test suite by introducing code mutations -> is it sensitive enough?
  - Rebuild testing: Delete src/, check if code behavior can be reproduced from specs and tests pass

Security, privacy, and legal aspects

Security aspects

- Privileges: With AI agents using tools, they can execute destructive actions on your PC
  - rm -rf / ?? - Antigravity https://news.ycombinator.com/item?id=46103532 , https://support.google.com/gemini/thread/415523107?hl=en
- Tool and API manipulation:
  - Modify tool / API to trigger unauthorized action, ie. an MCP server bcc'd email content to an external domain https://snyk.io/blog/malicious-mcp-server-on-npm-postmark-mcp-harvests-emails/
- Skill manipulation:
  - Skill file appears legitimate but contains malicious payload (Typosquatting, Memory poisoning, ClickFix prompts), ie. targeting crypto wallets and ssh credentials https://owasp.org/www-project-agentic-skills-top-10/ast01
- Prompt injection
  - For example, payload splitting - malicious content is divided in multiple prompts
- Secrets leakage
  - Can happen without intent - .env file in your project folder?

Privacy: https://copilot.github.trust.page/faq

- User Engagement Data: accepted or dismissed completions, error messages, system logs, and product usage metrics (stored for two years)
- Prompts: inputs for chat or code along with context (not retained)
- Suggestions: AI-generated code lines or chat responses provided to users (not retained)
- Feedback Data: real-time user feedback, including reactions (e.g., thumbs up/down) and optional comments, along with feedback from support tickets (“stored for as long as needed for its intended purpose”)
- Data from individual licenses (ie, student licenses) is used for training (not the case for GitHub Enterprise or Business) - same as with other providers

Legal aspects

- If you incorporate third-party code, you need to make sure there are no license incompatibilities
- However, with Copilot you may use another person's code unaware
- How will you provide attribution/copyright?

GitHub is being sued because of this
https://hackernoon.com/doe-vs-github-ammended-complaints-on-copyright-infridgement-open-source-licenses-and-more

You may block suggestions that match public code, but this only works from 150+ characters (ignoring whitespace).

Feature providing a reference to matching public code
https://github.blog/2022-11-01-preview-referencing-public-code-in-github-copilot/

Legal aspects

Who owns the code that your agent created?

Copyright: Protects your intellectual property right in software creation:

But: If the agent wrote the software, is it still *your* code?

>>> the US Copyright Office has confirmed that copyright protection requires human authorship, and that material generated by AI without sufficient human creative control is not registrable. In particular, they have noted that when a complex work is made by a prompt, “these prompts function more like instructions to a commissioned artist”, with the result uncopyrightable.<<<

https://www.twobirds.com/en/insights/2026/belgium/ai-coding-can-you-protect-what-your-agents-create
https://www.copyright.gov/ai/

Ethical aspects

- Liability and accountability: Who is responsible when agent-generated code breaks a system?
- Attribution: How do you properly attribute AI-written code?
- Bias: What about niche frameworks / languages?
- Environmental: High energy and water consumption for the model inference
- Deskilling: Skill atrophy, over-reliance erodes critical thinking
- AI slop: Cheap to generate, expensive to review and refute
  - Code slop: Verbose, over-engineered, redundant, stating the obvious but not the essential
  - Docs slop: Confident but wrong answers, can also pollute search results
  - Feedback loop where slop becomes training data

Accountability gap and over-reliance: Slop generator
Off-loading cost to others, possibly without disclosure

Human review
Disclose AI use
Quality gates

Beyond the technical

Engineeringification

Trend that traditionally non-technical roles adapt engineering mindset

Example: Design engineer, Growth Engineer, Prompt Engineer, Support Engineer

➢ adopt engineering-style processes, tools, and mindsets and prioritizing data, automation, and structured systems over purely qualitative work

Reason: Tools become more powerful, and LLMs make them more accessible; and people identify more with what they are building and who they are building it with.

https://posthog.com/newsletter/engineeringification-of-everything

The future of research?

Impact on research and the research process

Powerful tools put even more knowledge at your fingertips - and can also break it down for you!

There are multiple levels of tools to support your work, from a chatbot, to an AI agent, to an AI agent using YOUR tools - for example, via an MCP.

+ Could allow you to spend more time on the creative process
+ Could allow you to think more across disciplines and approaches
+ Could make your science more accessible to others
- Could restrict the creative process by implicit rules that are present
- Could limit your learning and in-depth understanding

Summary

Learning goals

- Use AI-assistance in a coding environment
- Know about the limitations of these tools
- Know how to adapt AI agents
- Know how to provide tools to AI agents
- Be aware of legal and ethical implications
- Be aware of privacy and security concerns in the use of such tools