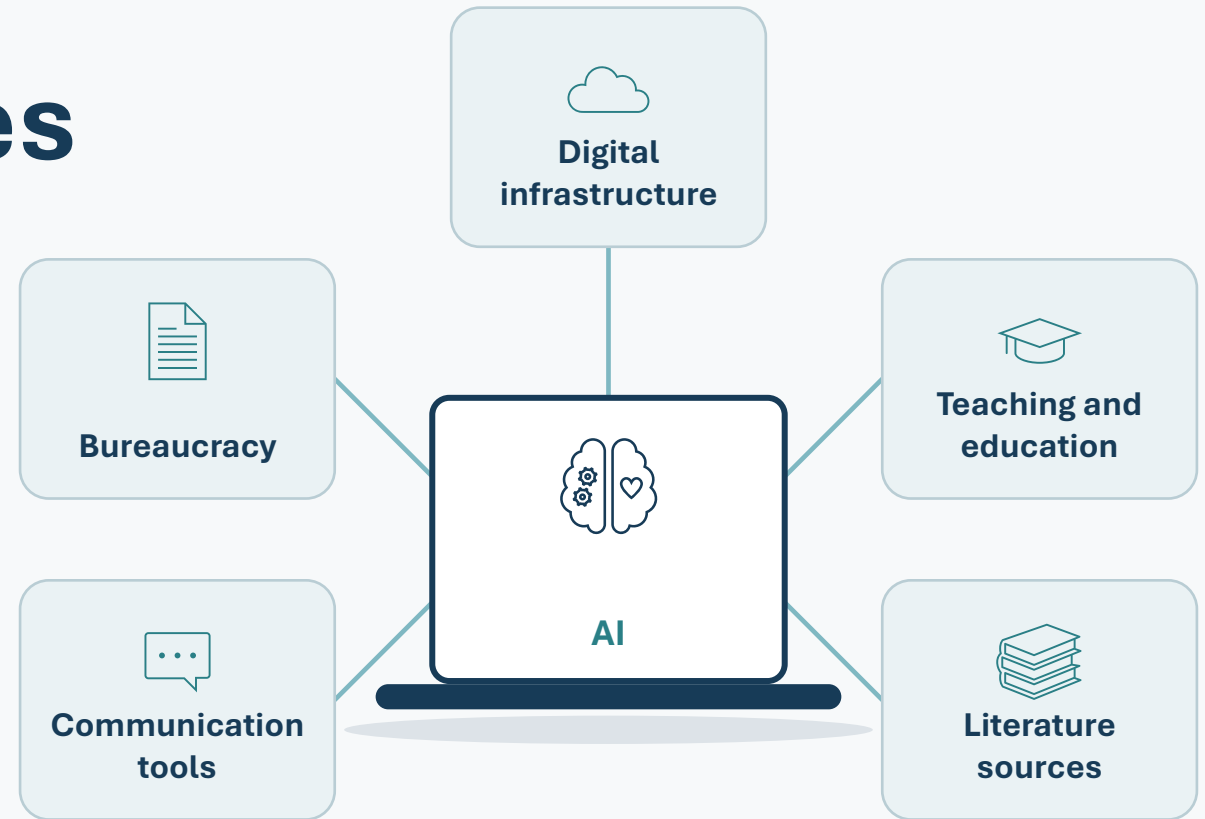


AI and Digital Services Available to Us

Tools you already pay for,
although you may not use them
(or may not even know they are there for you)



Academic digital workflow

Vojtěch Chlan | KFNT MFF UK

What We Will Cover Today



AI is a cross-cutting tool, not the seminar's only topic.

Will AI Replace You, or Will Someone Who Knows How to Use It?



(AI generated. No horse was harmed during the process.)

The part of the joke that holds

A better tool gives a real advantage –
to whoever uses it.

The relevant point

We all pay for it.

A few use it.

The rest fund their advantage.

How Do We Use AI Today?

“How do you currently use generative AI or large language models?” · N = 25, status 5 October 2026

Not at all

never tried, or tried briefly and stopped

Occasionally

a chatbot for basic tasks

Regularly

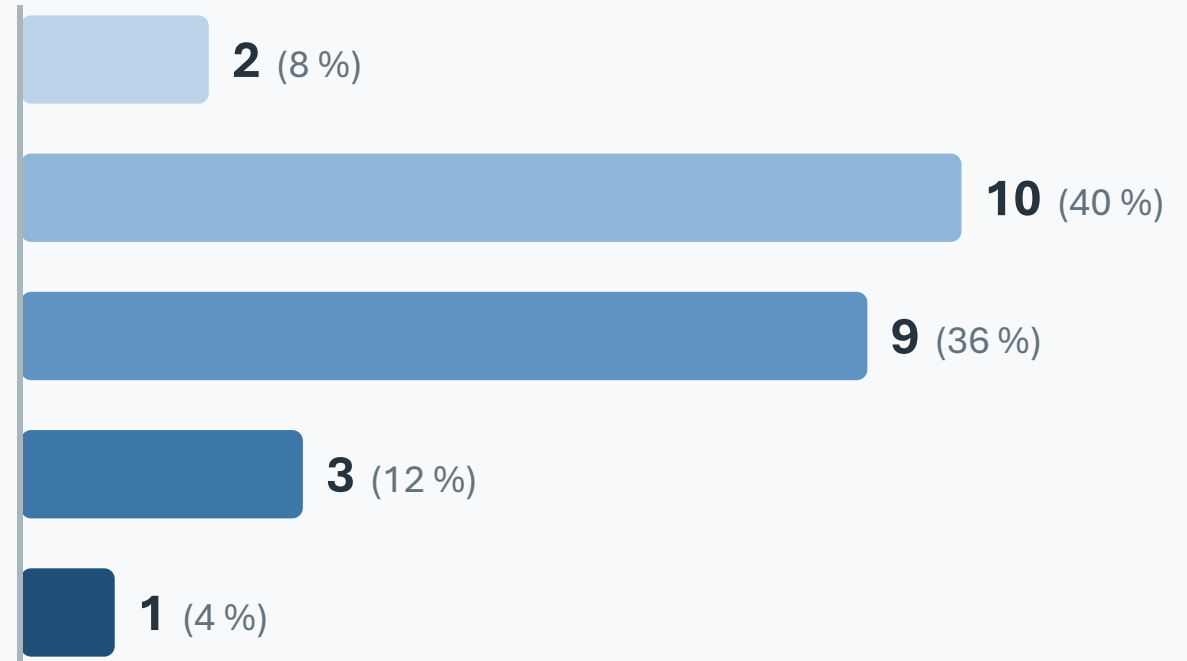
AI for several types of work

Part of my normal workflow

frequent use, specialised tools or integrations

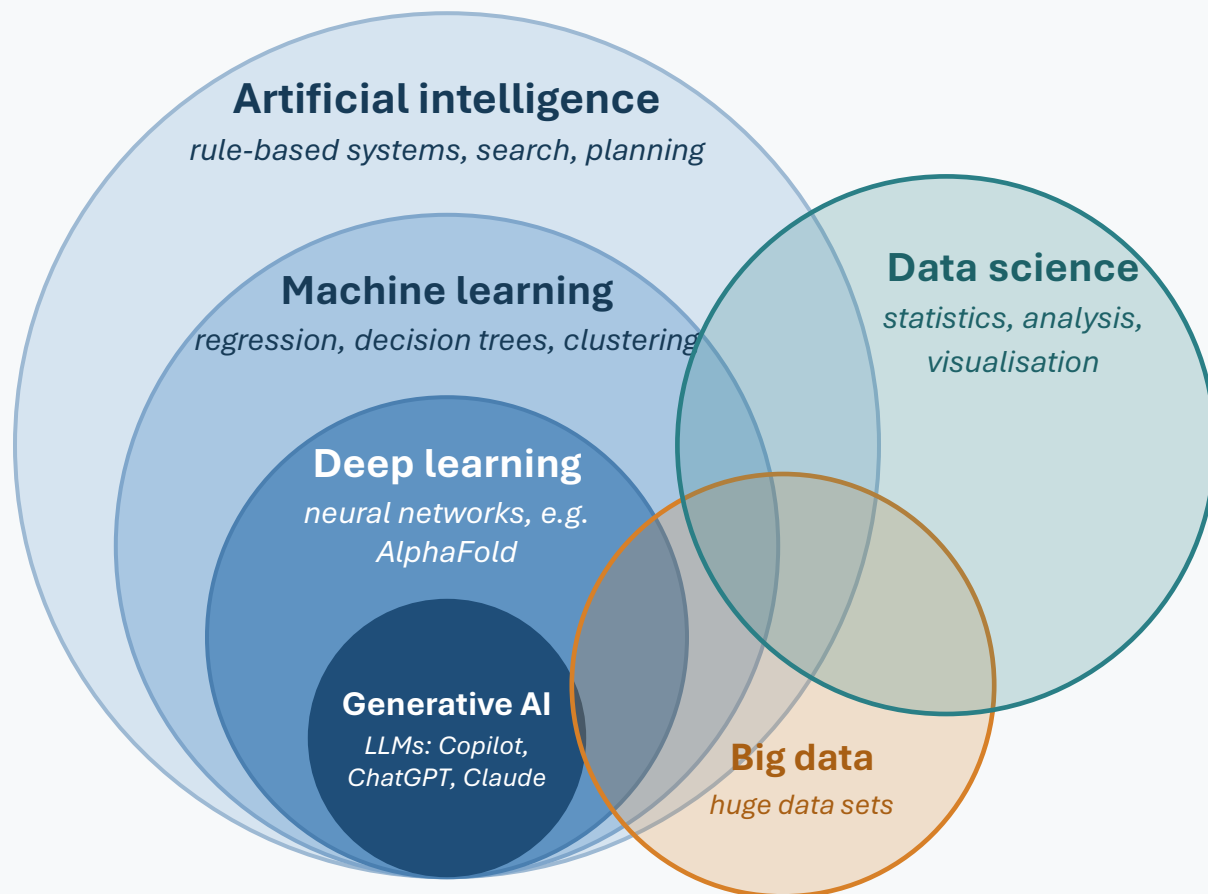
Very extensively

agents, CLI tools, APIs, advanced integrations



Roughly half of us use AI regularly, the other half only occasionally or not yet.

AI, Machine Learning, Data Science: How They Relate



Artificial intelligence

machines doing tasks we associate with intelligence – also without learning

Machine learning

rules learned from data instead of written by hand

Deep learning

machine learning with many-layer neural networks

Generative AI, LLMs

deep learning that produces text, images or code

Data science

knowledge from data: statistics + programming + domain expertise – uses ML, but not only

Big data

data too large for ordinary tools – distributed storage and computing; feeds large models

Copilot, ChatGPT and Claude sit in the smallest circle – AI is much broader.

Even Experts Can Find New Technology Overwhelming

“

I have always wished that my computer would be as easy to use as my telephone.

My wish has come true.

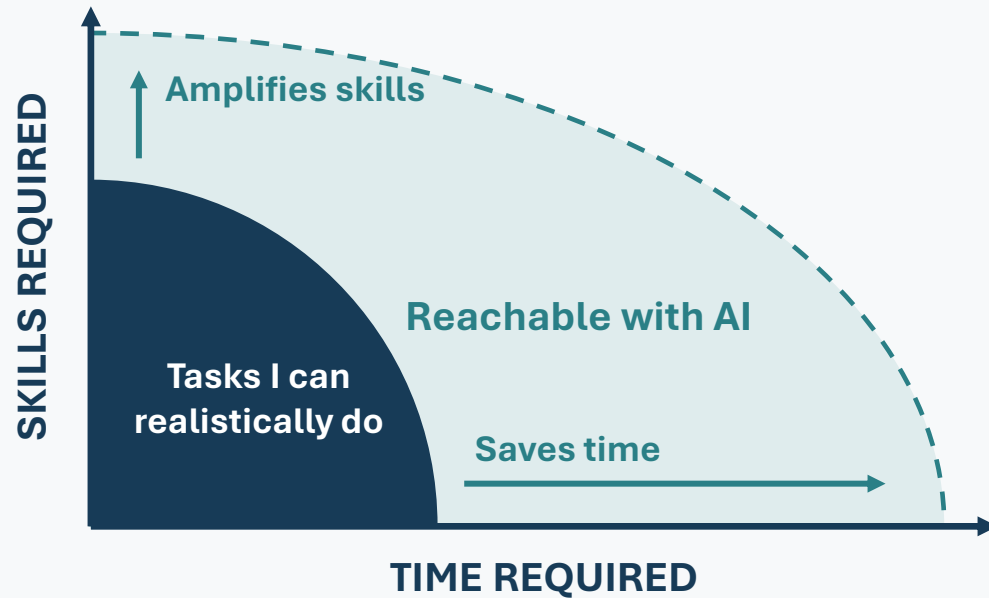
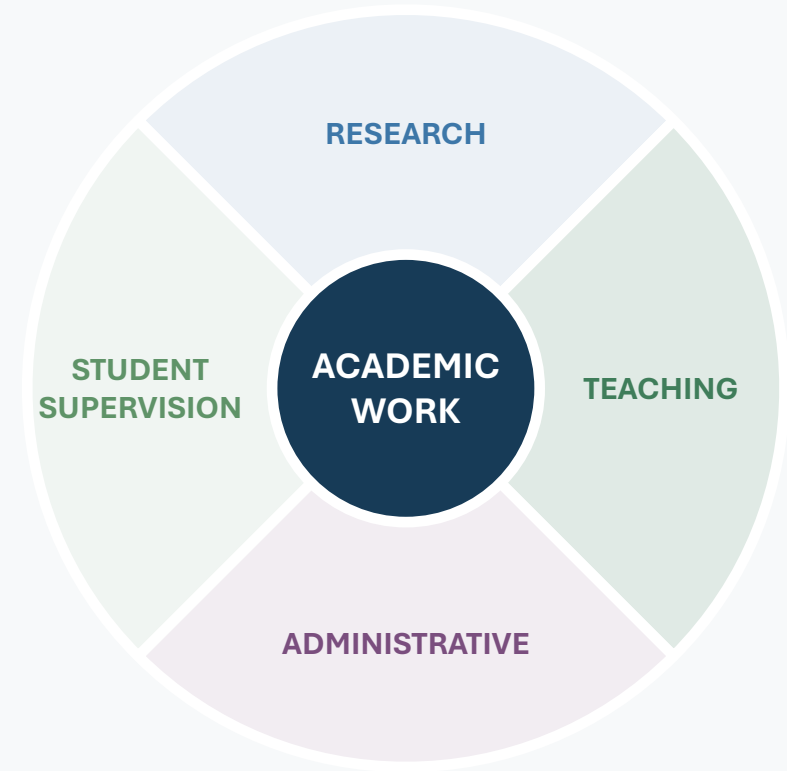
I no longer know how to use my telephone.

— Bjarne Stroustrup



Natural language lowers the initial barrier. It does not remove the need to understand the result.

Two Useful Schemes for This Seminar



AI can save time, help with difficult tasks,
or leave more time for checking.

Less time on routine work = more time for the creative one

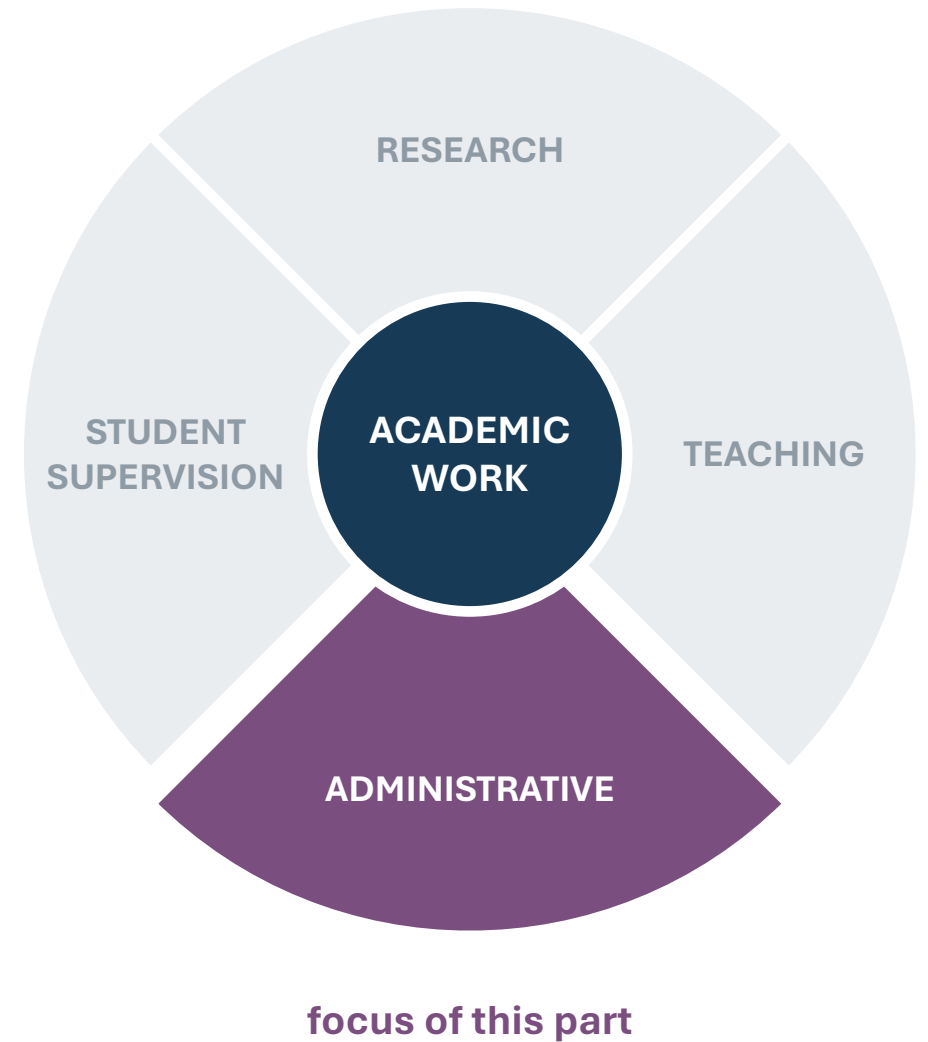
In all four areas of our work, AI can widen what we can realistically do.

PART 1

Administration and Documents

Where our time disappears · what is inside an AI assistant ·
finding rules · comparing versions · everyday text work

Live demos D-01 · D-02



Where Does Our Time Disappear Without Adequate Value?

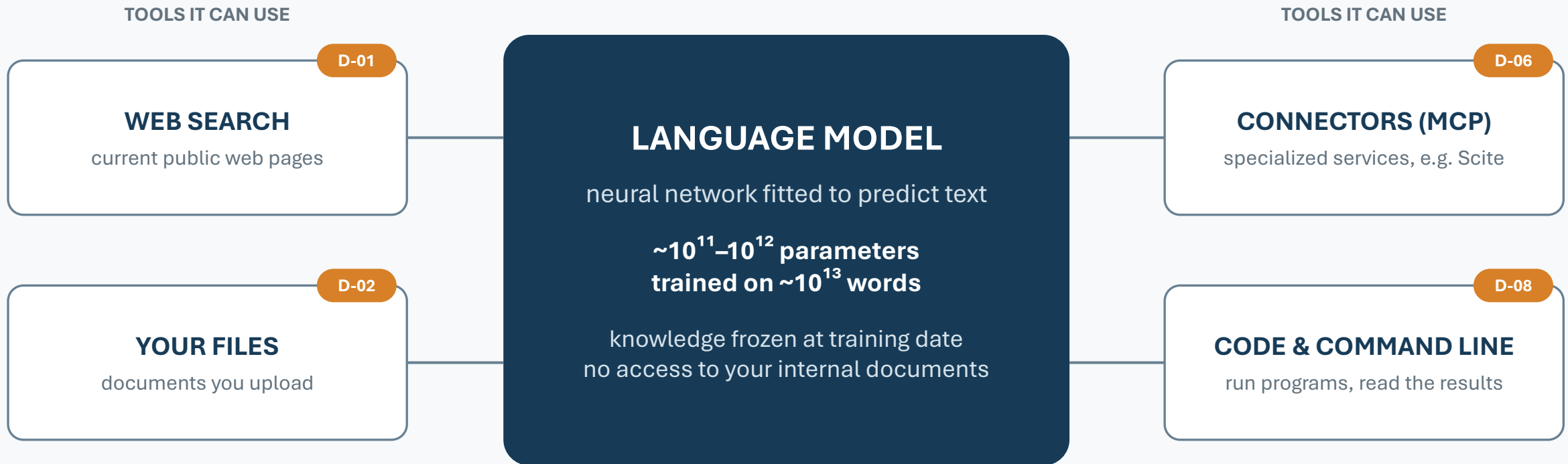


(AI generated. No physicist was harmed during the process.)

- Finding internal rules and procedures
- Reading long documents
- Comparing annual versions
- Summarizing email threads
- Drafting, translating, and recording text
- Filling out forms

Start where AI is strong and unlikely to take away the intellectually interesting part of the job.

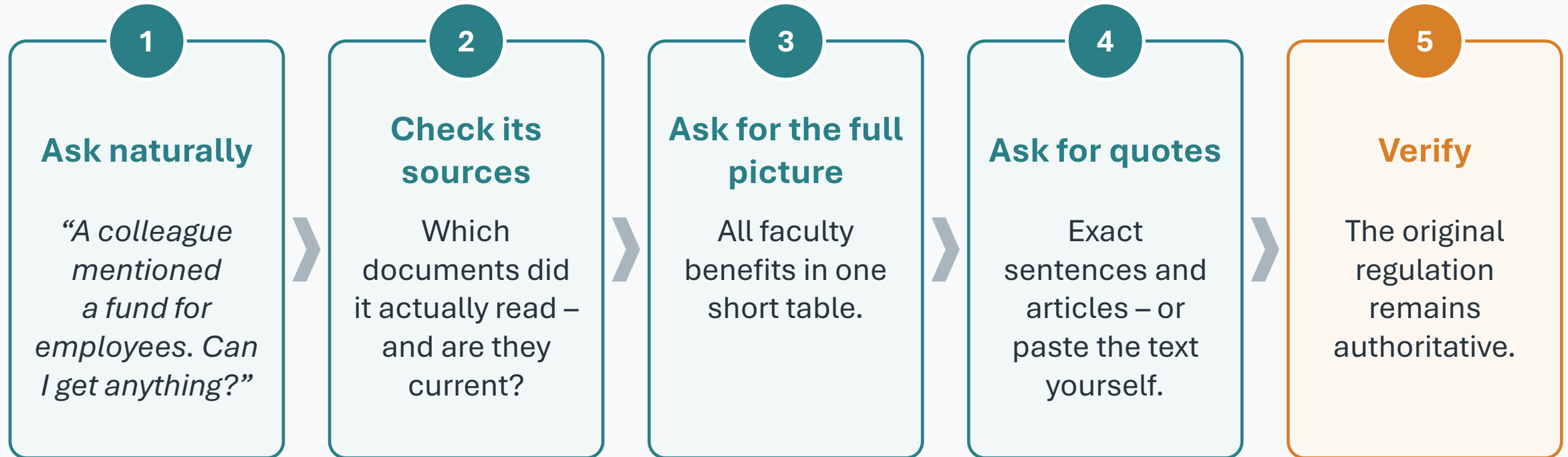
What Is Inside an AI Assistant?



e.g. Llama 3.1 (open model, 2024): **405 B parameters** in **126 layers** · each token = **16 384 numbers** · vocabulary $\approx$ **128 000 tokens**

What the model can reach matters as much as what it remembers.

Social Fund: From a Vague Tip to a Useful Overview

[▶ LIVE DEMO D-01](#)

A vague question becomes a useful overview – once I check the sources and ask for quotes.

AI + Human + Verification

AI

Find connections
Structure information
Summarize and reformat

HUMAN

Provide working context
Supply internal sources
Assess relevance

CHECK

Open the original document
Locate the exact provision
Confirm it is up to date

The same model applies to literature, programming, and computation.

Two Document Versions: What Actually Changed?

[▶ LIVE DEMO D-02](#)

GA ČR Standard Projects – call documentation 2026 vs 2027 (83 pages each, in Czech)

WEAK PROMPT

“Compare these documents.”

in my test runs:

- ✓ found the biggest change
- ✗ long text, no table
- ✗ no page numbers

BETTER PROMPT

- Substantive changes only
- Answer in English
- One narrow table with pages
- Impact and certainty
- Fewer rows is fine

→ an answer I can check

MY CHECK

Run 1	■	■	■	■	■	■	■
Run 2	■	■	■	■	■	■	■

correct · partly / duplicate · wrong

Every wrong row was labelled
certainty “high” or “medium”.

Each run gave different rows.

A better prompt makes the answer checkable – not automatically correct.

How to Assign a Task to AI

GOAL

What do I want to achieve?

CONTEXT

Why do I need it, and for whom?

SOURCES

What should the tool work from?

OUTPUT

What should the result look like?

CHECK

How should uncertainty be handled?

Treat it like a new assistant, not an oracle.

Other Everyday Text Work

EMAIL THREAD

Summary, action items, and a draft reply.

TRANSLATION

Terminology, tone, alternatives,
and ambiguous passages.

DICTATION

Spoken sentence → immediate
transcription.

PERSONALIZATION

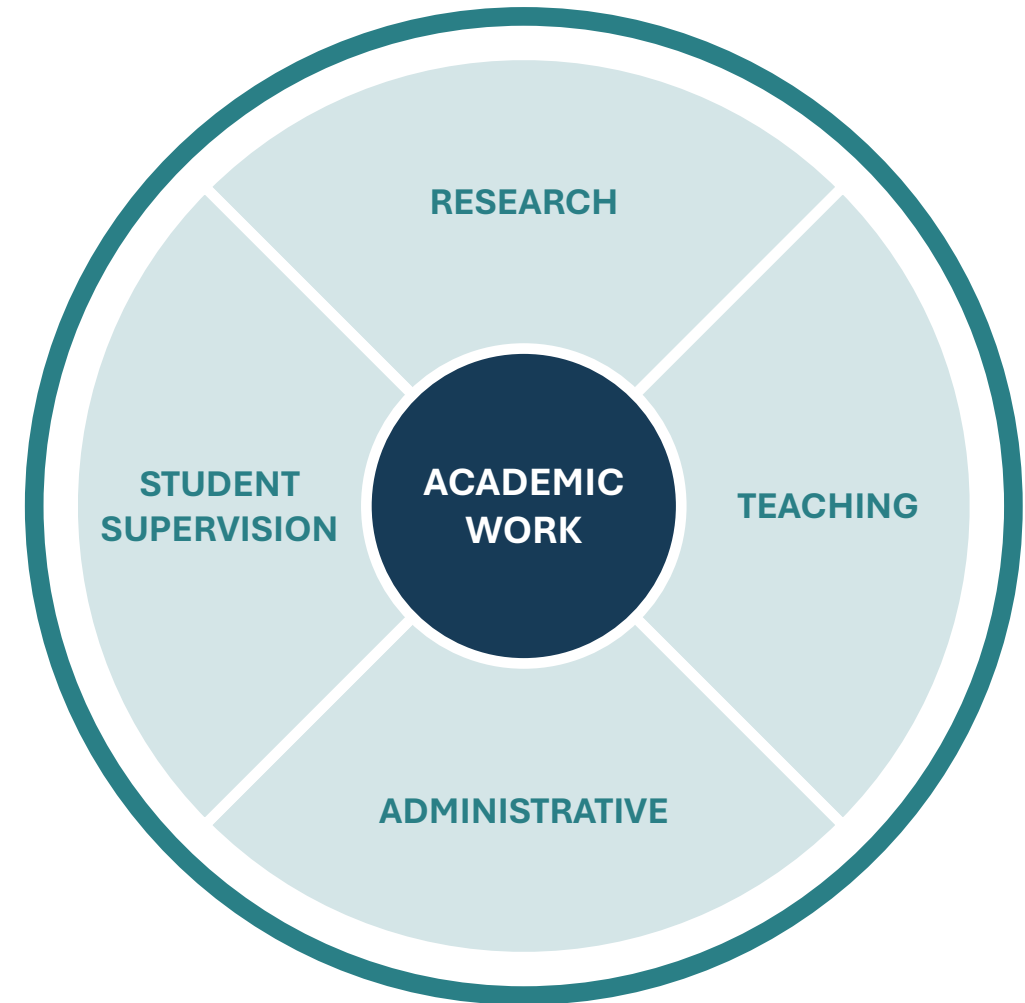
Preferences, history, and available context.

PART 2

Services and Infrastructure

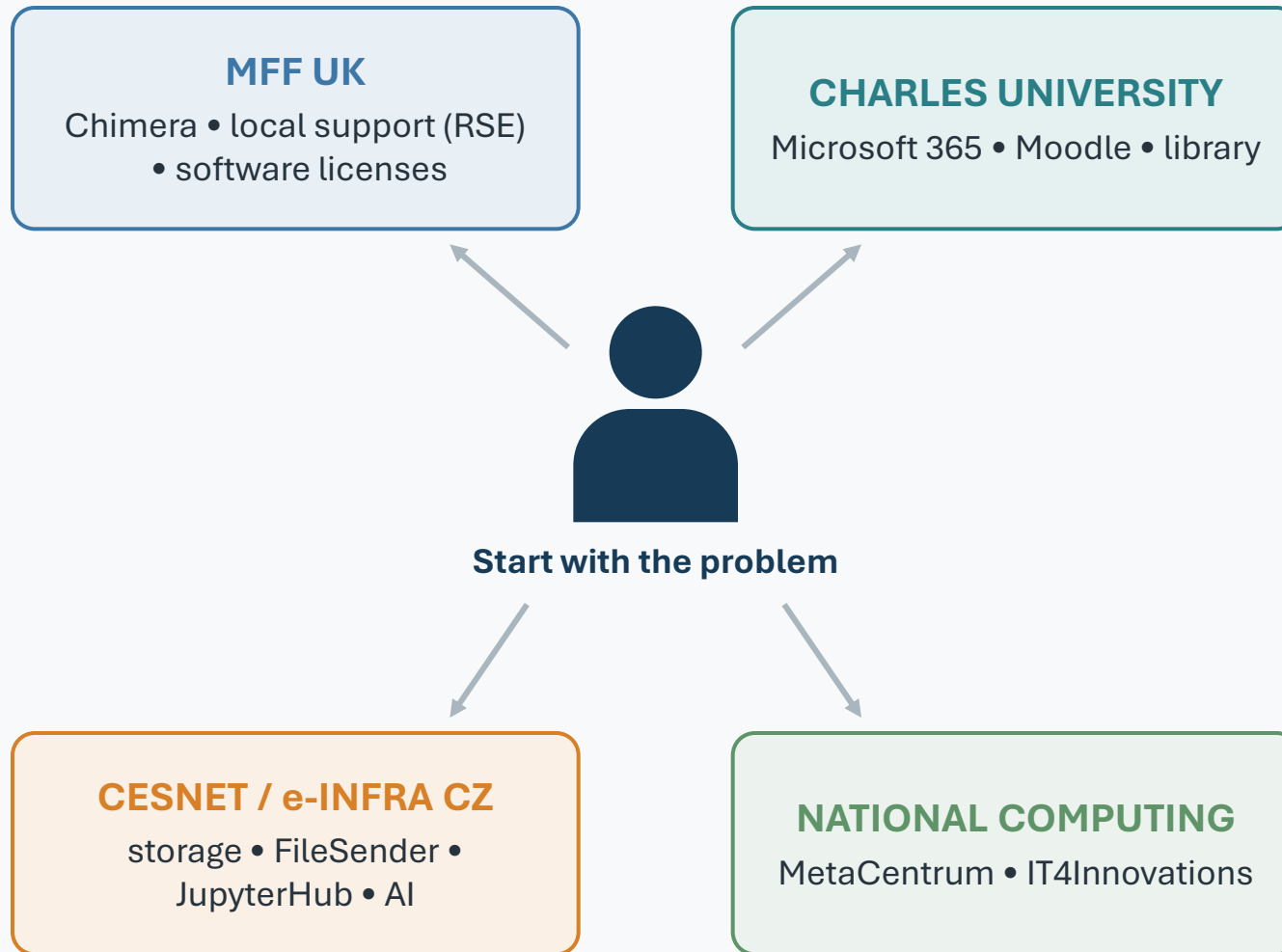
Who provides what · e-INFRA CZ · storage, sync and backup · a real backup case

Live demos D-03 · D-04



infrastructure supports all four areas

A Fragmented Ecosystem of Services



- Different providers and access routes
- Information spread across several websites
- The user needs a starting point, not an organizational chart
- A useful question:
What problem am I trying to solve?

Start with the problem you need to solve, not with the organizational structure.

One Starting Point: e-INFRA CZ Documentation

[▶ LIVE DEMO D-03](#)

Account

Access and identity

2 Data processing

MetaCentrum, IT4I,
cloud, Kubernetes

1 Storage

S3, Onedata,
OwnCloud, FileSender

Web services

JupyterHub, Galaxy,
Open OnDemand

Collaboration

Polls, Matrix, Slido,
Overleaf

3 AI as a service

Chat, API, MCP,
coding assistants

Start from the problem, not from the service list:

1 big file to send → FileSender 2 bigger calculation → MetaCentrum 3 AI chat, data stays in CZ → Chat AI

Storage, Synchronization, Transfer, and Backup Are Different

SYNC

Working files
across devices

OneDrive
OwnCloud

TRANSFER

Deliver a large file

FileSender

BACKUP

Scheduled,
versioned copy

Duplicati + storage

OBJECT STORAGE

Scalable storage
interface

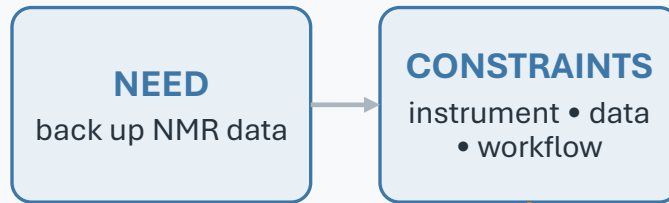
S3 and other uses

A synchronized cloud folder is not automatically a reliable backup.

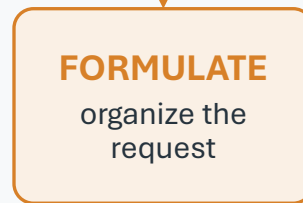
Automatic Backup in Practice

▶ LIVE DEMO D-04

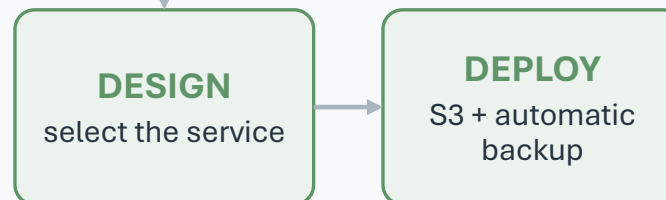
LABORATORY



AI SUPPORT



CESNET



- Automatic and scheduled
- Low-maintenance
- Encrypted where appropriate
- Last successful run is visible
- Restore must be tested
- **Storage can fail too**

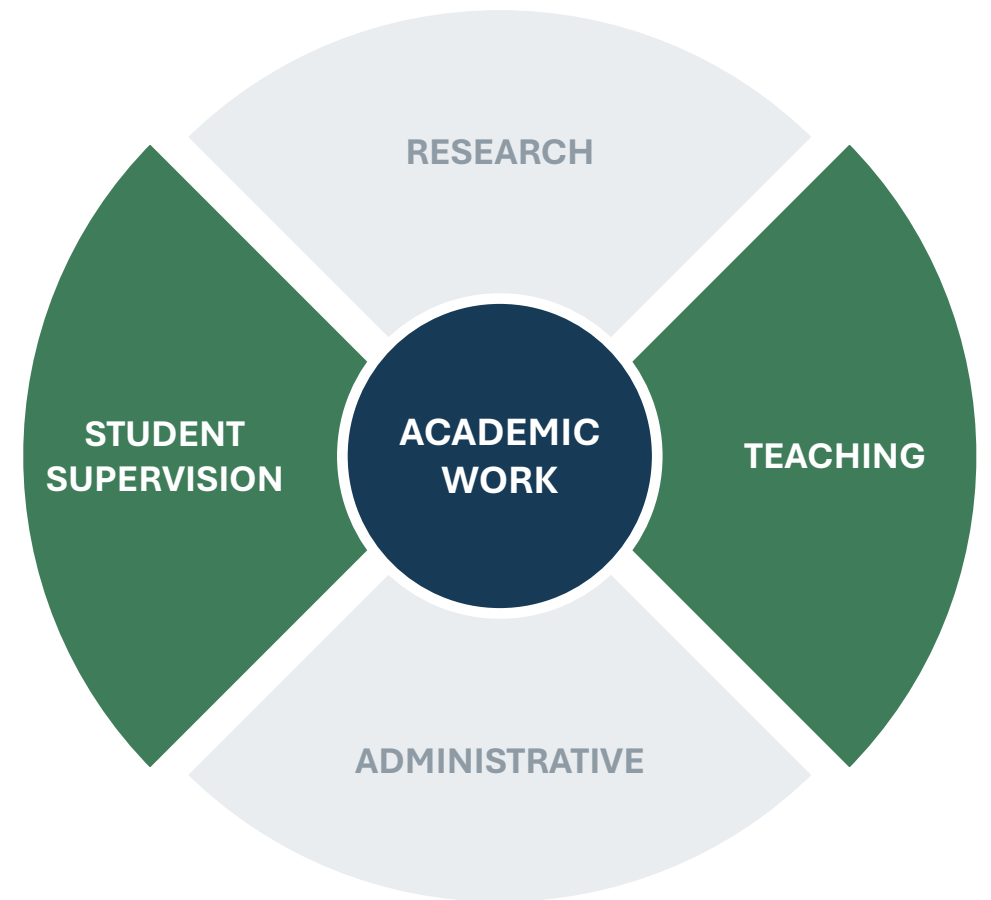
AI helped formulate the problem. CESNET experts designed and verified the solution.

PART 3

Teaching and Students

Course design · exercises · supervision · shared writing in Overleaf

Live demo D-05



focus of this part

Teaching and Student Supervision

COURSE DESIGN

Update a syllabus

Compare objectives with
actual materials

Restructure older content

EXERCISES

Generate variants

Check units and
consistency

Draft assessment rubrics

SUPERVISION

Plan milestones and work
plans

Prepare consultation
agendas

Keep track of agreed next
steps

Expert supervision and responsibility for assessment remain human.

AI helps me organise – it does not talk to students or read their theses for me.

One Shared Writing Environment

[▶ LIVE DEMO D-05](#)

```
\subsection{DFT calculations and hyperfine  
fields}
```

First-principles calculations were used to assign the measured `\mn` NMR spectra to local Mn environments. Rather than relying on absolute resonance frequencies, we use the calculated relative hyperfine-field shifts, site multiplicities, and number of nonequivalent Mn sites to identify signatures of antisites, APB-like environments, and martensitic modulation.



2.3. DFT calculations and hyperfine fields

First-principles calculations were used to assign the measured ^{55}Mn NMR spectra to local Mn environments. Rather than relying on absolute resonance frequencies, we use the calculated relative hyperfine-field shifts, site multiplicities, and number of nonequivalent Mn sites to identify signatures of antisites, APB-like environments, and martensitic modulation.

To model the electronic structure of Ni_2MnGa , we utilized density functional theory calculations using the all-electron full-potential linearized augmented plane-wave + local orbitals method as implemented in the WIEN2k

4th September, 5:21 pm

Edited
main.tex

■ You

4th September, 5:14 pm

Edited
main.tex

■ You

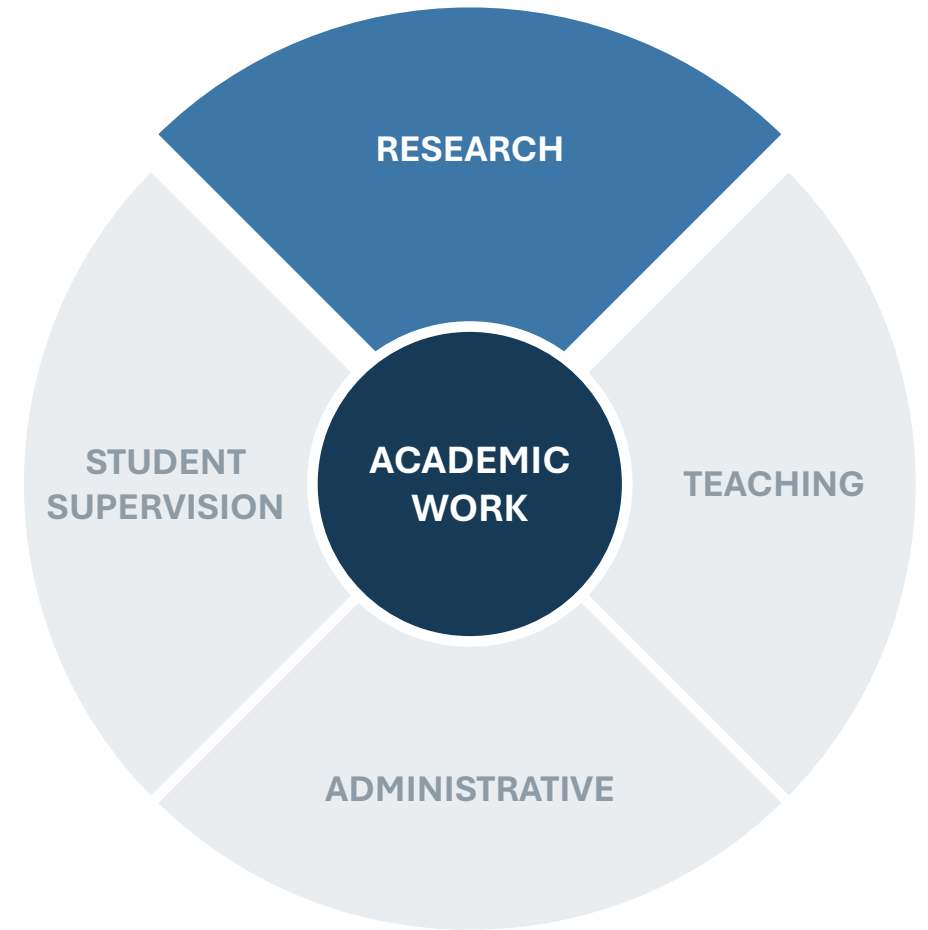
- | | |
|--|-----------------------|
| • LaTeX source and compiled PDF side by side | as in TeXstudio |
| • Co-editing, comments, track changes | as in MS Word |
| • Writefull AI language and grammar check | <i>built in</i> |
| • Full version history and easy sharing | <i>on top of both</i> |

PART 4

Research

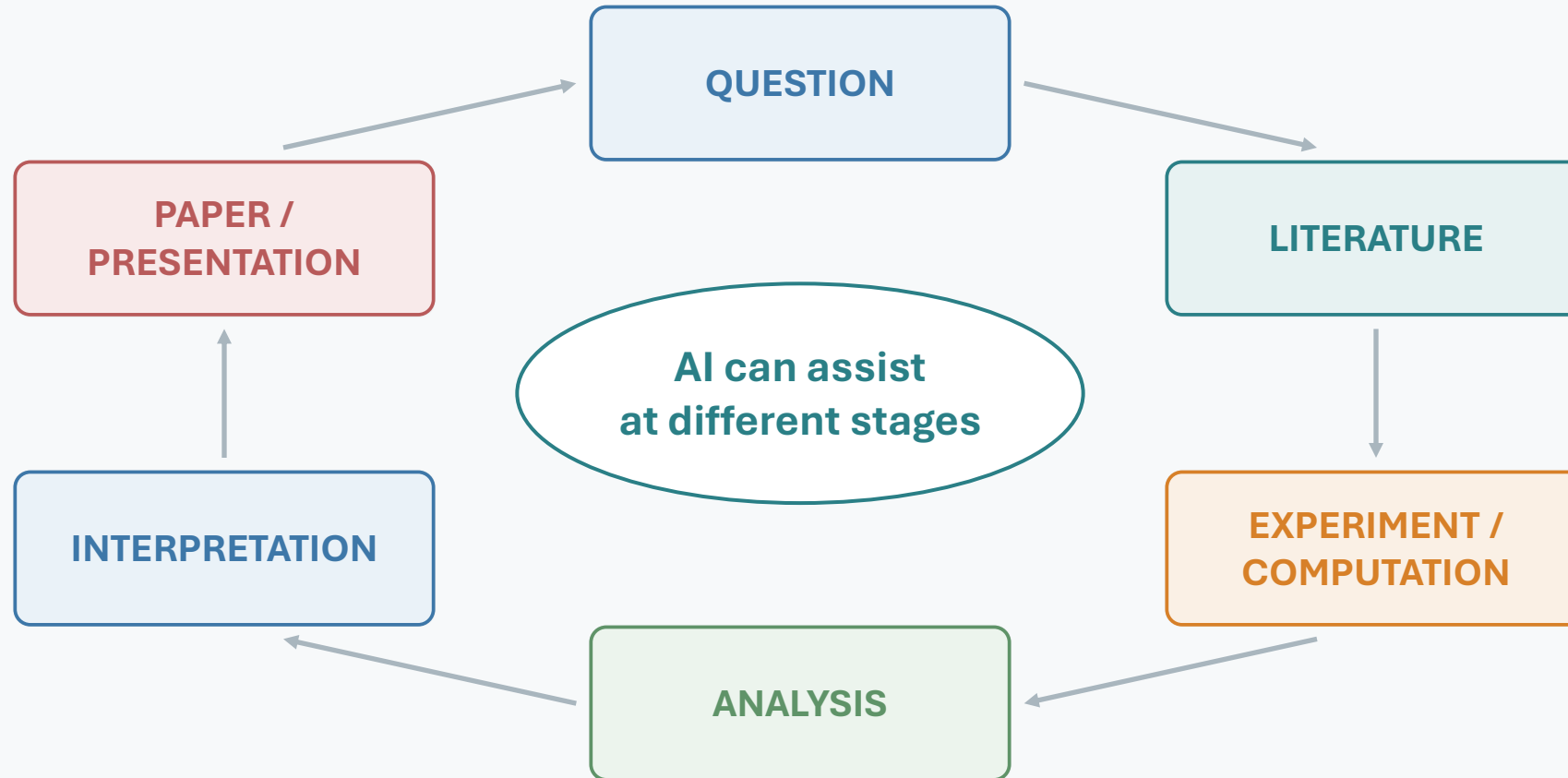
Research cycle · literature with Scite · computing resources ·
AI-assisted programming · when answers are wrong

Live demos D-06 · D-07



focus of this part

From a Research Question to a Publication



AI can assist across the cycle, but reliability and acceptable risk differ at each stage.

Three Ways to Work with Scite

[▶ LIVE DEMO D-06](#)

1 USE SCITE DIRECTLY

I describe the search directly in Scite.

Useful, but writing an effective query can be difficult.



2 LLM WRITES THE PROMPT

I explain what I am looking for in ordinary language.

A general LLM turns it into a better Scite prompt.



3 LLM CALLS SCITE

Scite is connected to the general LLM through MCP.

The LLM formulates and runs the search in one conversation.

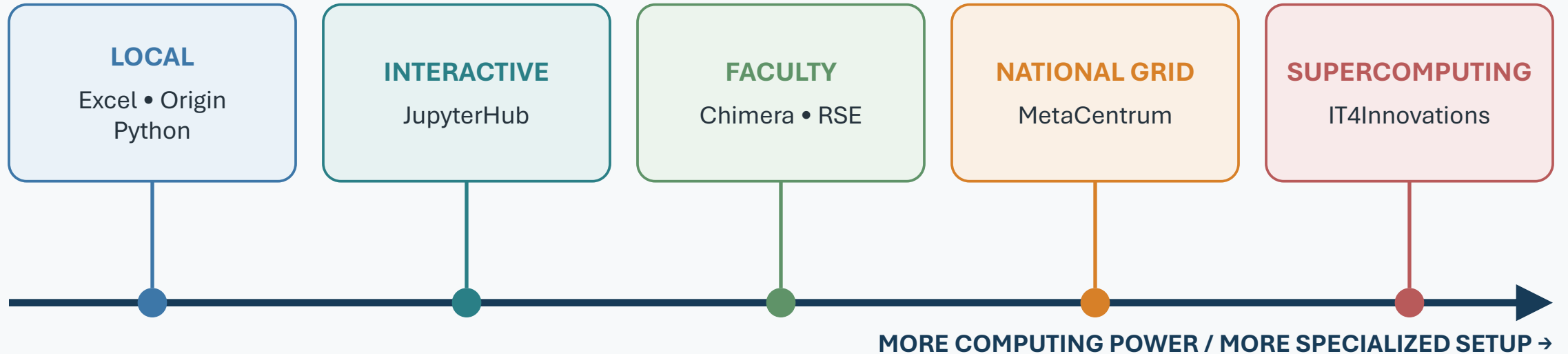
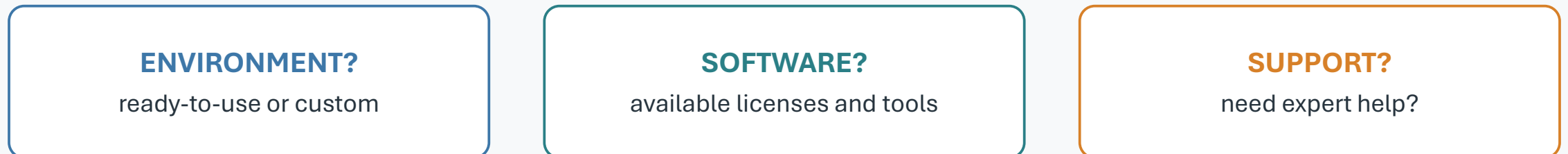
Claude: direct connector

Copilot: agent in Copilot Studio

A general LLM can translate my intent into the language of a specialized tool.

From a Laptop to a Supercomputer

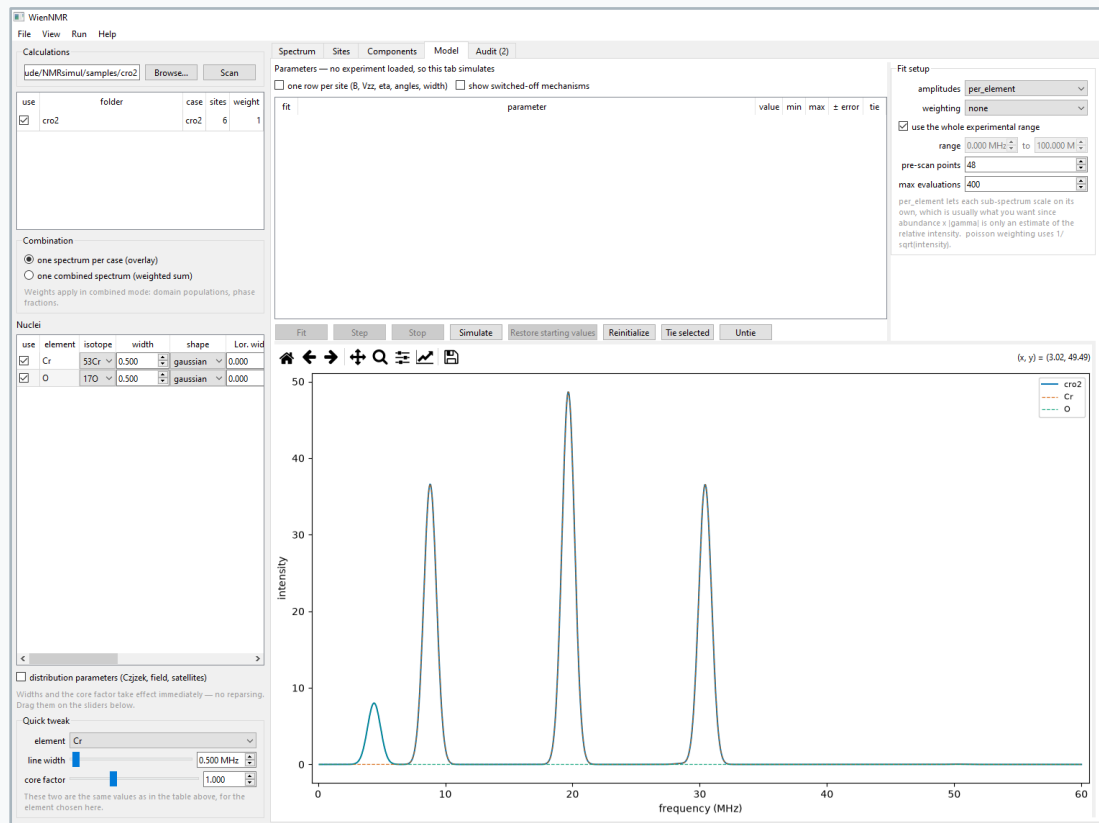
IF TIME D-03 continued



If time: back to the e-INFRA CZ and MFF UK pages – what can I actually compute there?

Choose the level that matches the problem.

A Program I Could Not Have Written Efficiently on My Own



WienNMR: WIEN2k output → NMR sites → spin Hamiltonian → spectrum.
Replaces bash + Python script + Excel + Mathematica + Origin.

I DEFINE physics, units, conventions – in a written record

WienNMR – conventions and physics record

Anything that could be got wrong by a plausible-looking guess is written down here ...

AI HELPS BUILD code, explanations, reading WIEN2k Fortran

ROTATE PERFORMS A ROTATION OF THE VECTOR
FROM THE GENERAL CARTESIAN COORDINATION
SYSTEM INTO THE LOCAL ONE → $\mathbf{v}_{loc} = \mathbf{R} \cdot \mathbf{v}_{glob}$

WE TEST automatic self-check, run every session

ok sign of C_Q (of e, of V_{zz}) is not observable
ok engine reproduces legacy Mathematica spectrum
max deviation = **1.5e-14** of peak

Two AI mistakes caught and corrected: sign of e, first fit.

The useful result is not generated code. It is a tested, understandable tool.

Why I Often Prefer a Tested Tool to an Autonomous Answer

DIRECT AI DECISION

Fast and flexible

But intrinsically variable

May fail in a persuasive way

vs

AI-BUILT DETERMINISTIC TOOL

Specification + code + tests

Repeatable behavior

Easier to inspect and validate

Use AI to help build the method, then make the method reproducible.

A Trivial Question

▶ LIVE DEMO D-07

**How many days of the week
contain the letter d?**

Trivial for any of us. Will the language model get it right?

When a Plausible Answer Is Wrong

[▶ LIVE DEMO D-07](#)

PLAUSIBLE ANSWER

How many days of the week
contain the letter d?

**“Three: Wednesday,
Thursday, and
Saturday.”**

Copilot, answering straight away

INDEPENDENT CHECK

Write them out:

Mon-day · Tues-day
Wednes-day · Thurs-day
Fri-day · Satur-day
Sun-day

VERDICT

7 of 7

the answer was wrong

the model sees tokens, not letters

Language quality is not evidence quality.

Choose the check before asking whether the answer sounds convincing.

Three Rules for Responsible Use

SOURCE BEFORE ANSWER

For factual claims:
inspect the original and
authoritative source.

TEST BEFORE TRUST

For code and calculations:
use known cases, limits,
and independent checks.

RESPONSIBILITY STAYS HUMAN

AI does not assume
scientific, educational, or
institutional responsibility.

Before uploading anything to an LLM, assess the data:
public · internal · personal · confidential · unpublished · under review?

What We Have Access To

TOOL	WHAT FOR	DEMO	ACCESS
Microsoft 365 Copilot	everyday text work, documents, web search	D-01 · D-02	UK login
e-INFRA CZ / CESNET	storage, backup, computing, AI services	D-03 · D-04	e-INFRA CZ
Overleaf + Writefull	shared LaTeX writing, AI language check	D-05	UK licence
Scite	literature search with citation context	D-06	UK licence
Copilot Studio	your own agent, e.g. linked to Scite	D-06	UK login
Claude for Scientists	general LLM with connectors (e.g. Scite)		free on request

Outside the university login, other terms apply.

Check them before uploading internal, personal or unpublished data.

What to Try Tomorrow

- 1 NOTICE** one recurring task
- 2 CHECK** what is already available
- 3 TRY** one small real example
- 4 VERIFY** according to the risk
- 5 KEEP** what genuinely helps

A SIMPLE RULE

Low risk experiment freely

Higher risk verify more

Human interaction keep it human

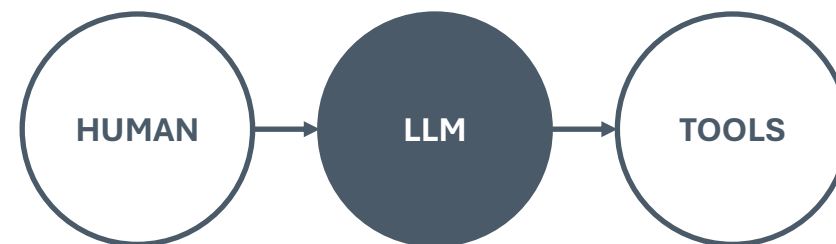
The point is not to fit more work into the same day. It is to leave more time for work that matters.

OUTLOOK · IF TIME ALLOWS

From Answers to Actions

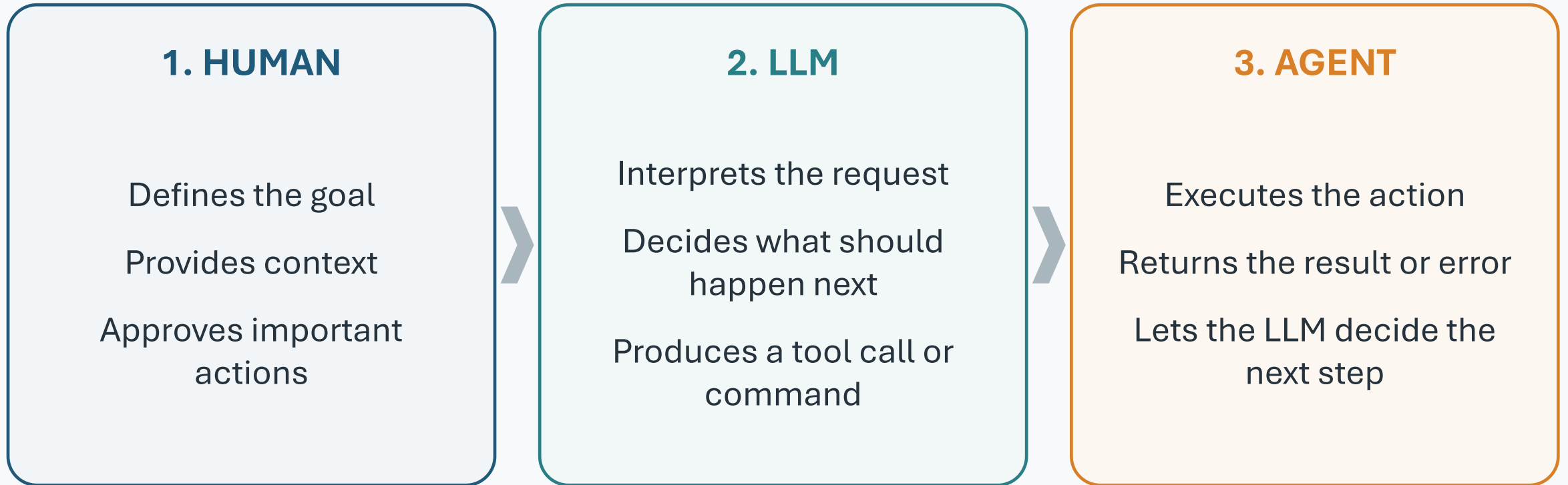
Agents · MCP and command line · safeguards · a lab
instrument driven from the command line

Live demo D-08



the model asks, tools act

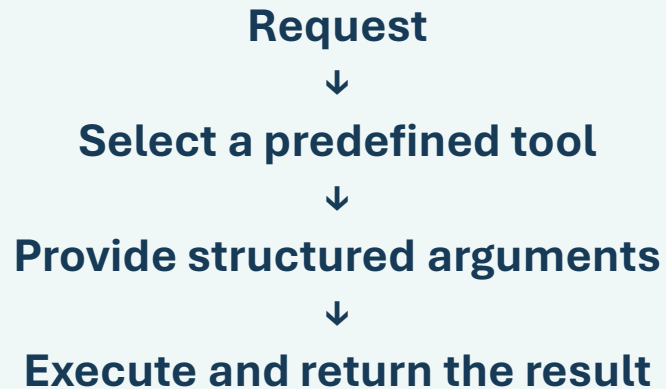
From Answering Questions to Taking Action



The LLM decides what to request. Another component performs the action.

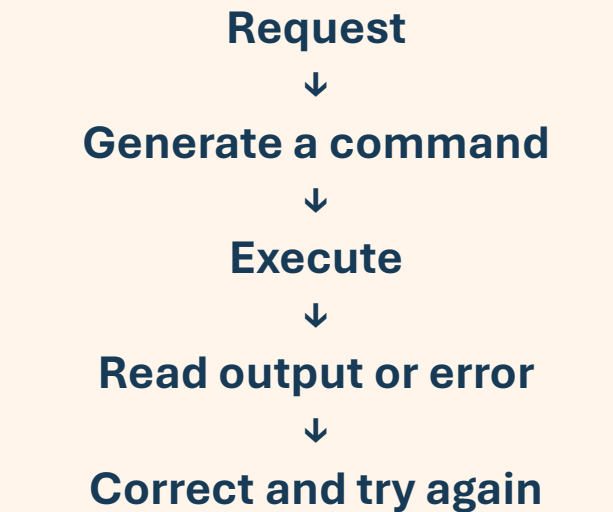
Two Ways for AI to Work with Other Tools

MCP: choose from defined tools



The available actions and their inputs are defined in advance.

CLI: issue a command and inspect the result



The model works step by step, using output and errors as feedback.

MCP constrains the available actions. CLI lets the AI work through the problem step by step.

Freedom Requires Safeguards

RESTRICT

Limit permissions

Allow only selected
commands or tools

ISOLATE

Use a sandbox

Keep experimental actions
away from important data

REVIEW

Use dry runs

Require confirmation for
consequential actions

More freedom makes the system more useful – and increases the need for control.

In practice: constrained tools combined with controlled command-line work.

Running a Mössbauer Lab from the Command Line

[▶ LIVE DEMO D-08](#)

GUEST DEMONSTRATION

Automating the lab workflow
an AI agent working on the command line

WHAT TO WATCH FOR

RESTRICT

Which commands or tools may the agent use?

ISOLATE

Where does it run, and which data can it touch?

REVIEW

Which steps wait for a human to confirm?

The model proposes commands – the safeguards decide what may run.