

TASCopilot: Architecture of an AI Research Assistant for Triple-Axis Neutron Scattering at NCNR

Aditya Purohit, Duke University

Mentor: Dr. William Ratcliff

NIST Center for Neutron Research

Previous Work – Summer 2025

- Prototyped this project
- Foundational architecture
- Basic Tools

Applications of Large Language Models and AI to Neutron Scattering



Aditya Purohit, Richard Montgomery High School

Mentor: Dr. William Ratcliff



National Institutes of Standards and Technology Center for Neutron Research

Video Demos:

This Summer - Acknowledgements



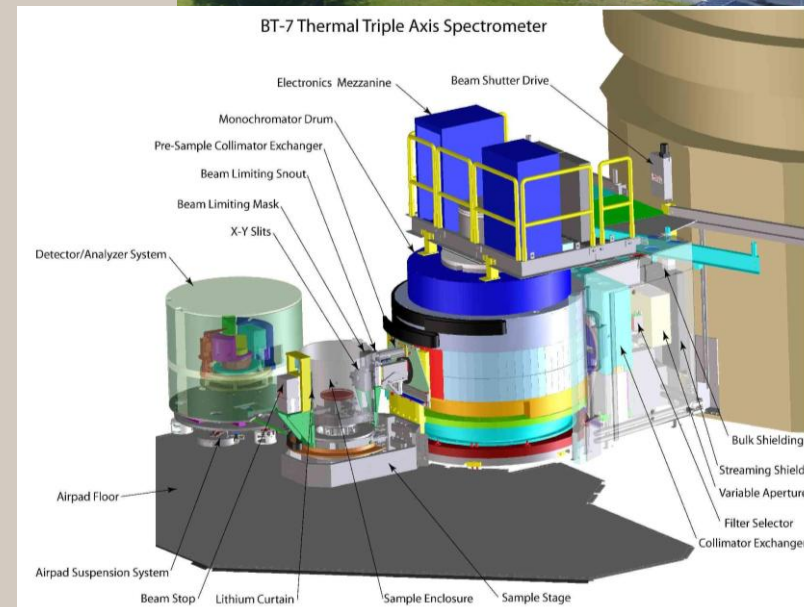
Srikar Kovvali

Dr. William Ratcliff

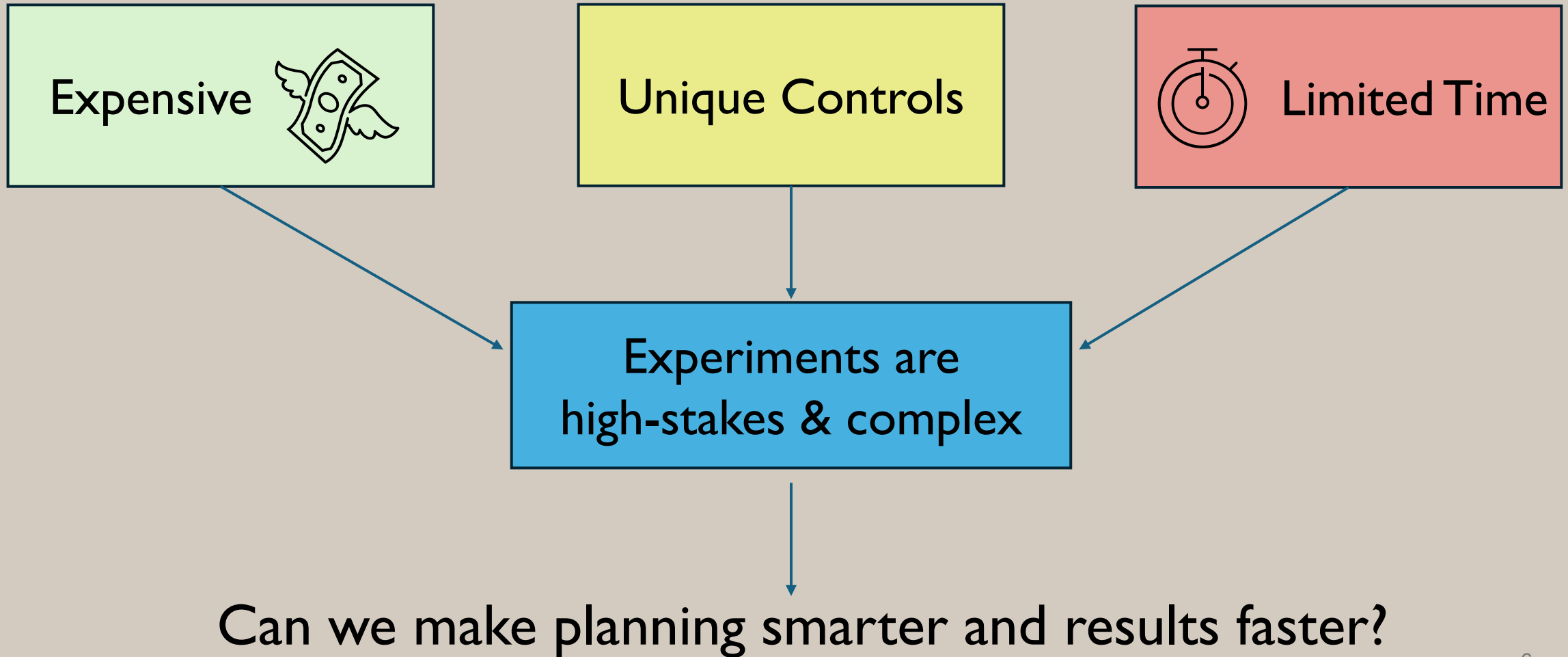
Carina Jacobson

The NCNR and Neutron Scattering

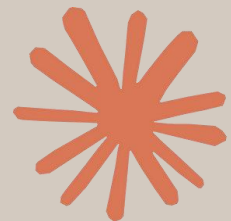
- User facility
- Shoots neutrons at samples
- One of many instruments: BT-7
 - To study structure & dynamics
- Superconductors, Thermoelectrics



The Problem



Everyone's First Idea

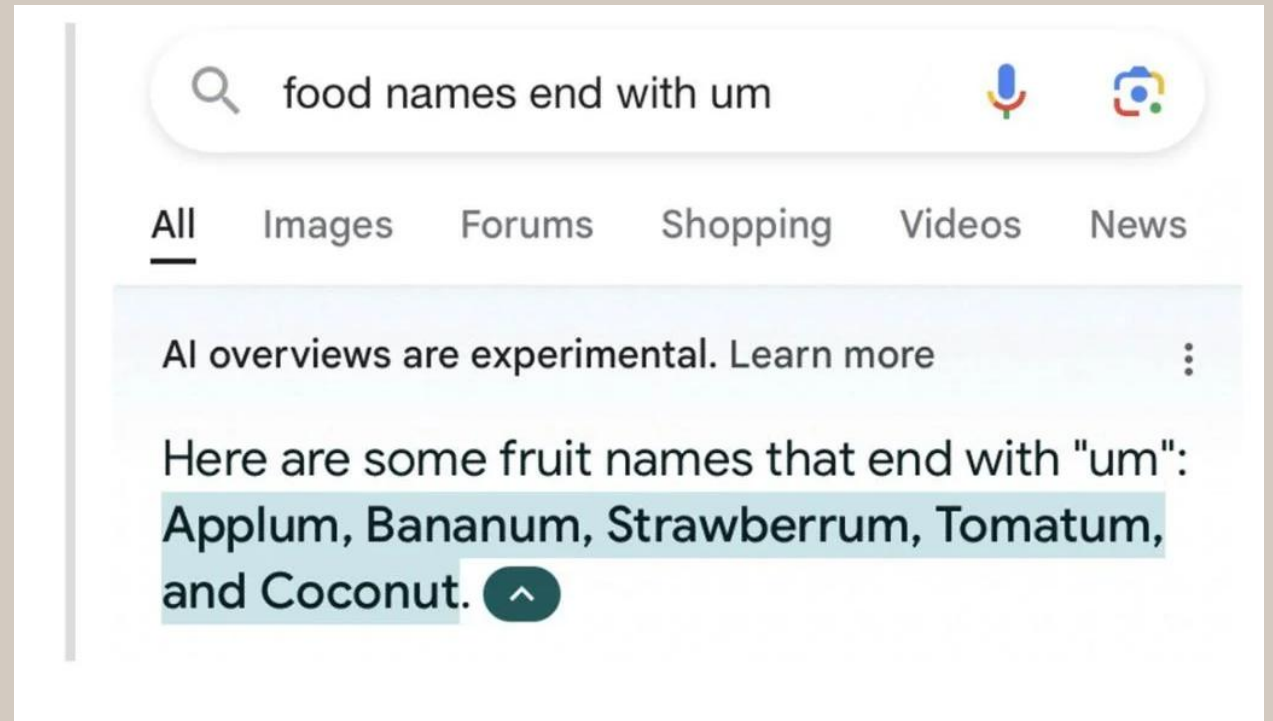
 Claude

 ChatGPT

 Gemini

 Grok

Problem



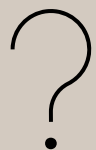
Lies, lies and more lies

Solution: (Triple Axis Spectrometer) TASCopilot

Generic Chatbots



Makes things up

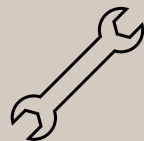


Unreliable Sources

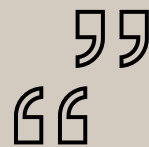


AI does everything

TASCopilot



Connects your tools



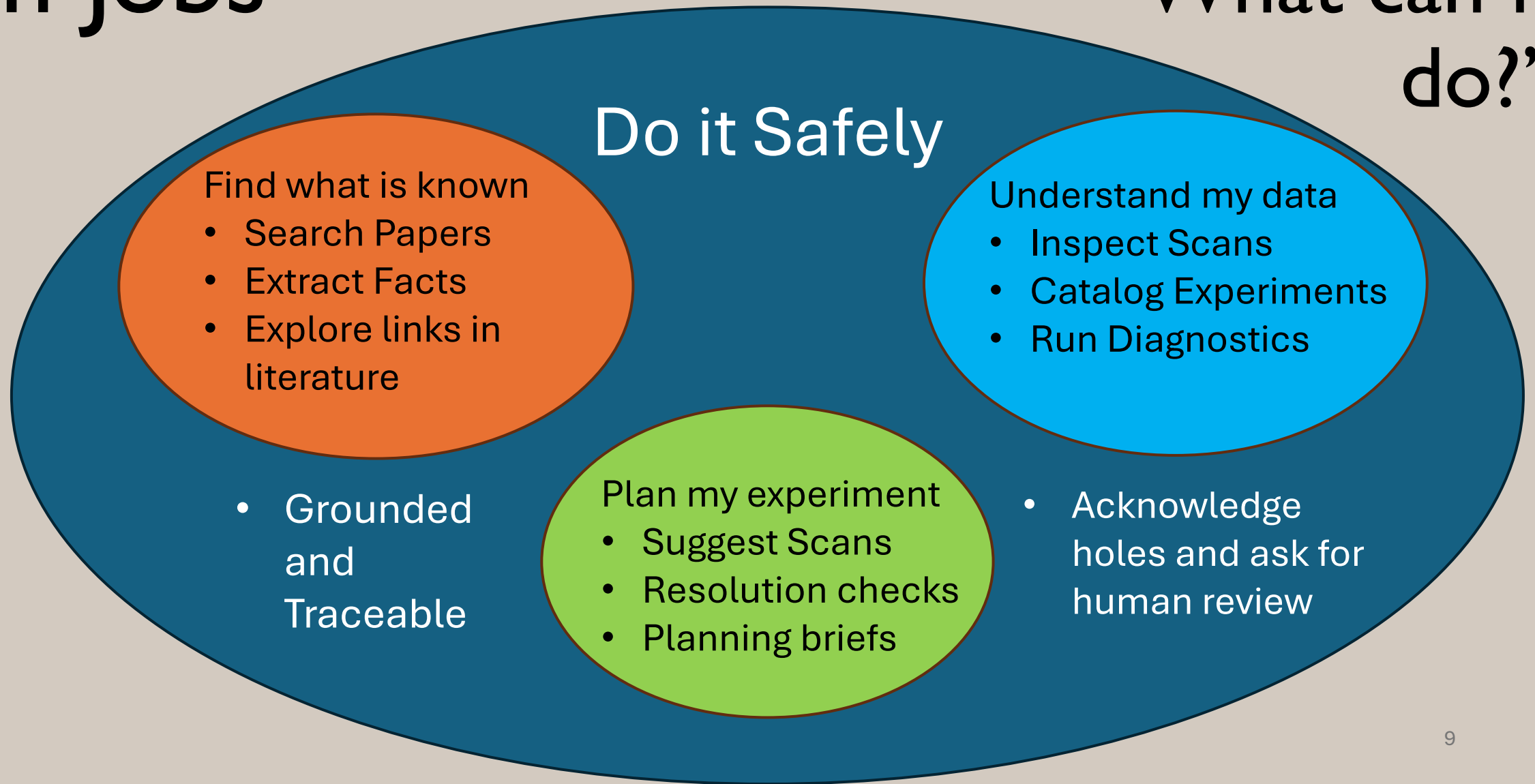
Grounded in real papers



Read-only Definition

Main Jobs

“What can it do?”



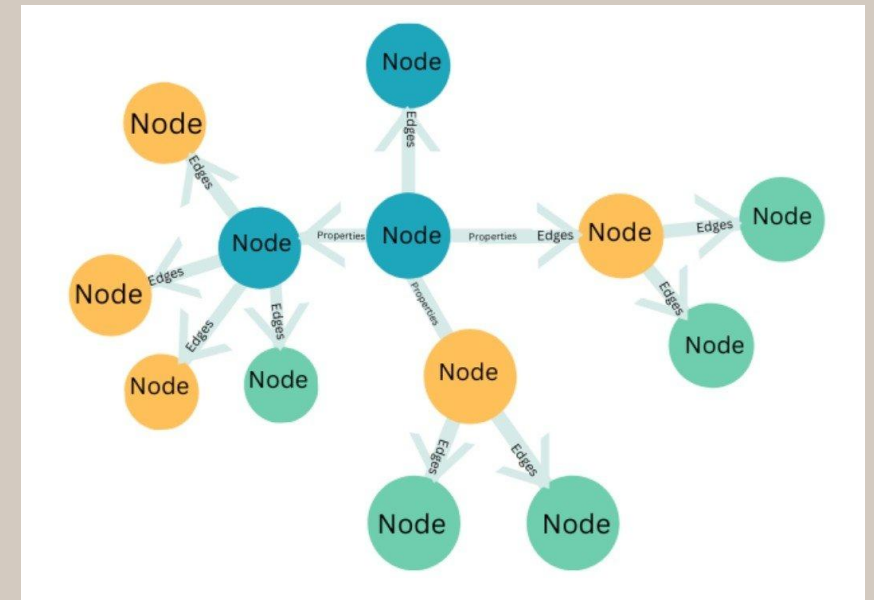
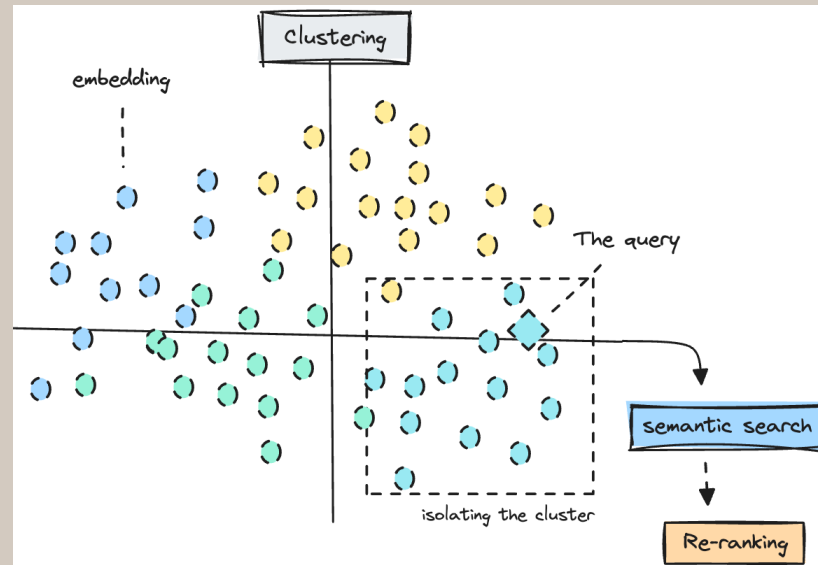
“Find What is Known”

Smart Search - 3 Parallel Strategies

Keyword Search

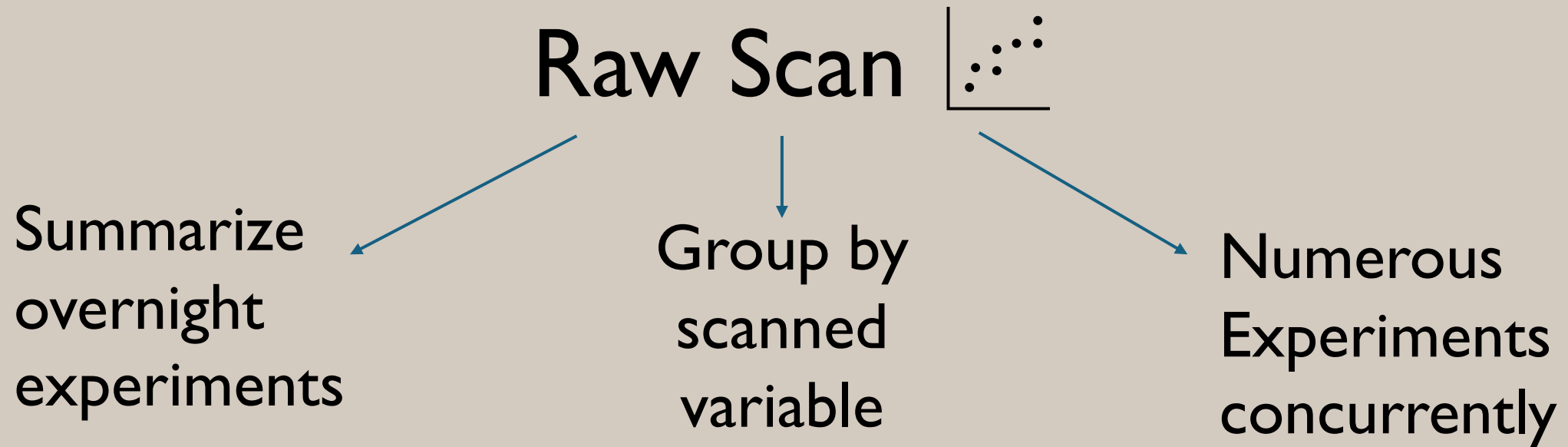
Semantic Search

Relationship Graph



“Understand my Data”

NLP, Metadata and Python



Copilot uses rules and metadata to determine the correct intention

“Plan my Experiment”

Data, NLP and Python



Inputs

- Literature
- Past experiments
- Structure factors
- Instrument limits

One Plan

- Staged scans
- Configs & temps
- Risks flagged
- Provenance present

Example

Use the paper_brief tool to summarize a paper. Set corpus_catalog to /home/anp27/tascopilot/local_runs/corpus_catalogs/bt7_corpus_since2015_vista_20260513_docling and paper_id to doc-28c3e16e9c3f

07/13/2026 at 1:22 PM

Use the corpus_question_answer tool to answer: What is SrMn₂Sb₂ and its general properties? Set corpus_catalog to /home/anp27/tascopilot/local_runs/corpus_catalogs/bt7_corpus_since2015_vista_20260513_docling



oi **gemma-4-31B-it**

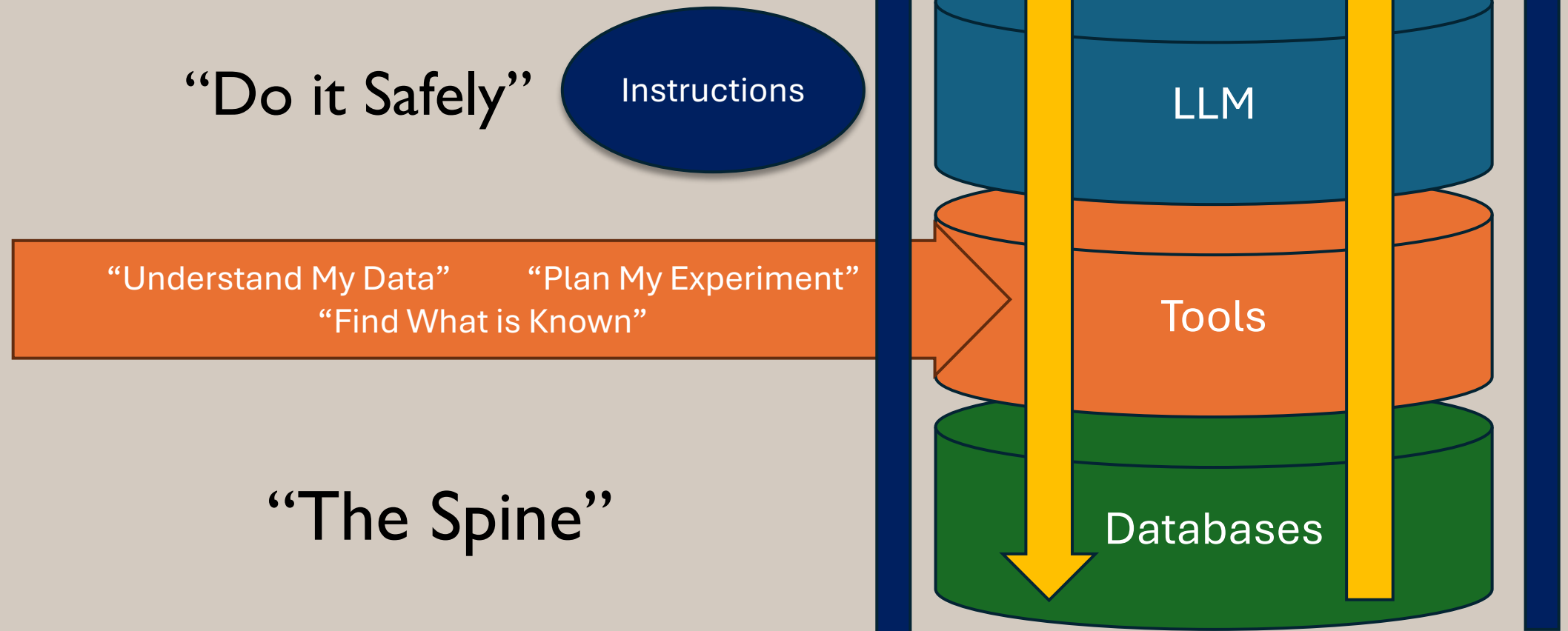
Based on the provided context, there is no specific information regarding the general properties of SrMn₂Sb₂. The retrieved excerpts mention other materials such as Fe₃Sn₂, TbMn₆Sn₆, and YMn₆Sn₆, as well as a reference to "Helical magnetism in Sr-doped" materials, but they do not contain details about SrMn₂Sb₂. server:0/tool_c...nswer_post

1 Source

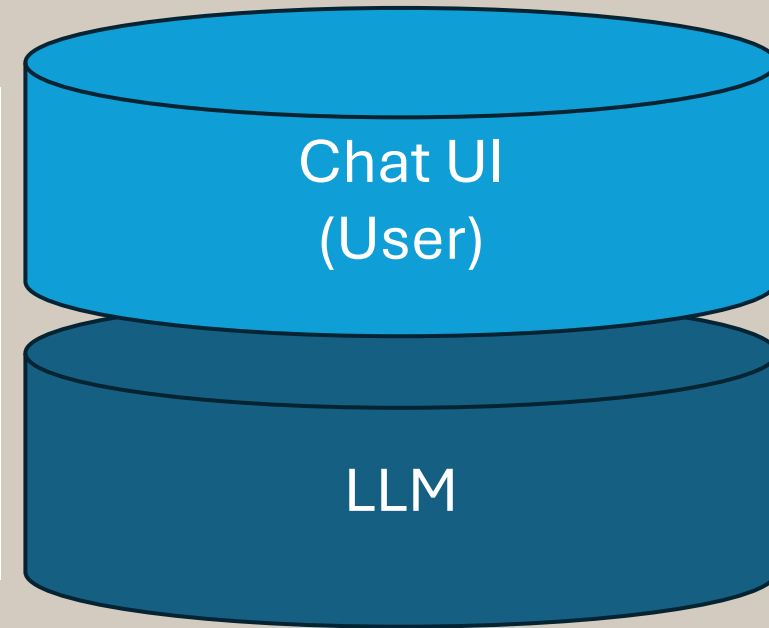
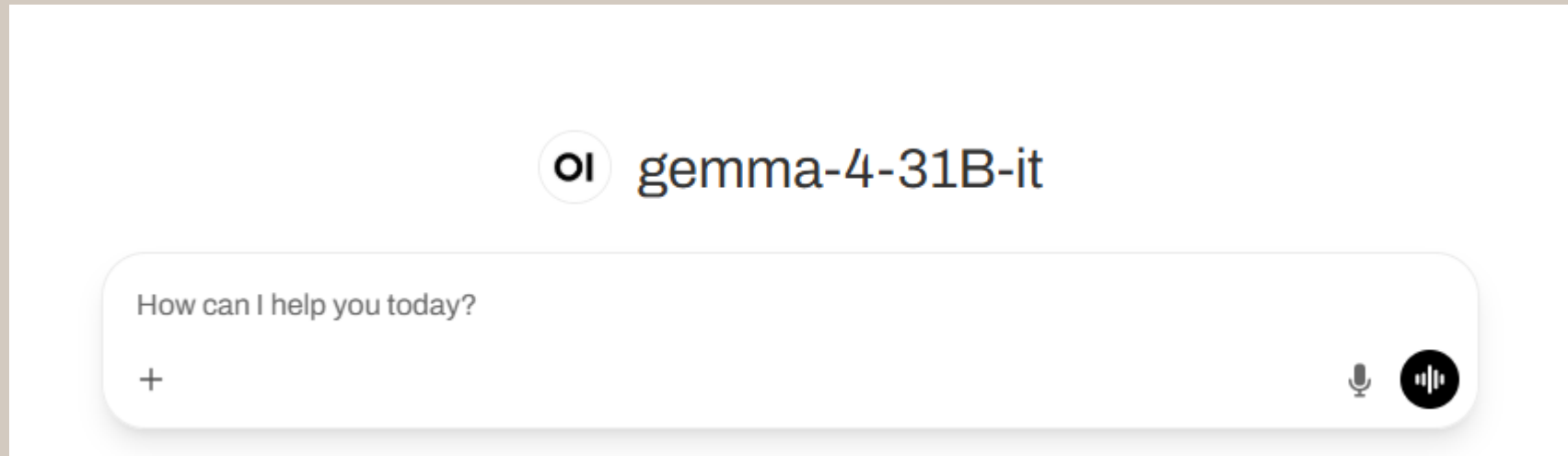
- The in-plane spontaneous anomalous Hall effect (AHE), $\rho_{zy}(B = 0)$, peaks near 30 K and decreases toward zero around 10 K. server:0/tool_paper_brief_post
- Magnetic Bragg peak analysis at $Q = (0001)$ indicates that the magnetic domain size ξ along y undergoes hysteretic changes under up-and-down sweeps of $B \parallel x$ at 2 K, with ξ being strongly reduced when the field is raised from zero to 4 T. server:0/tool_paper_brief_post

The Architecture

“How does it work?”



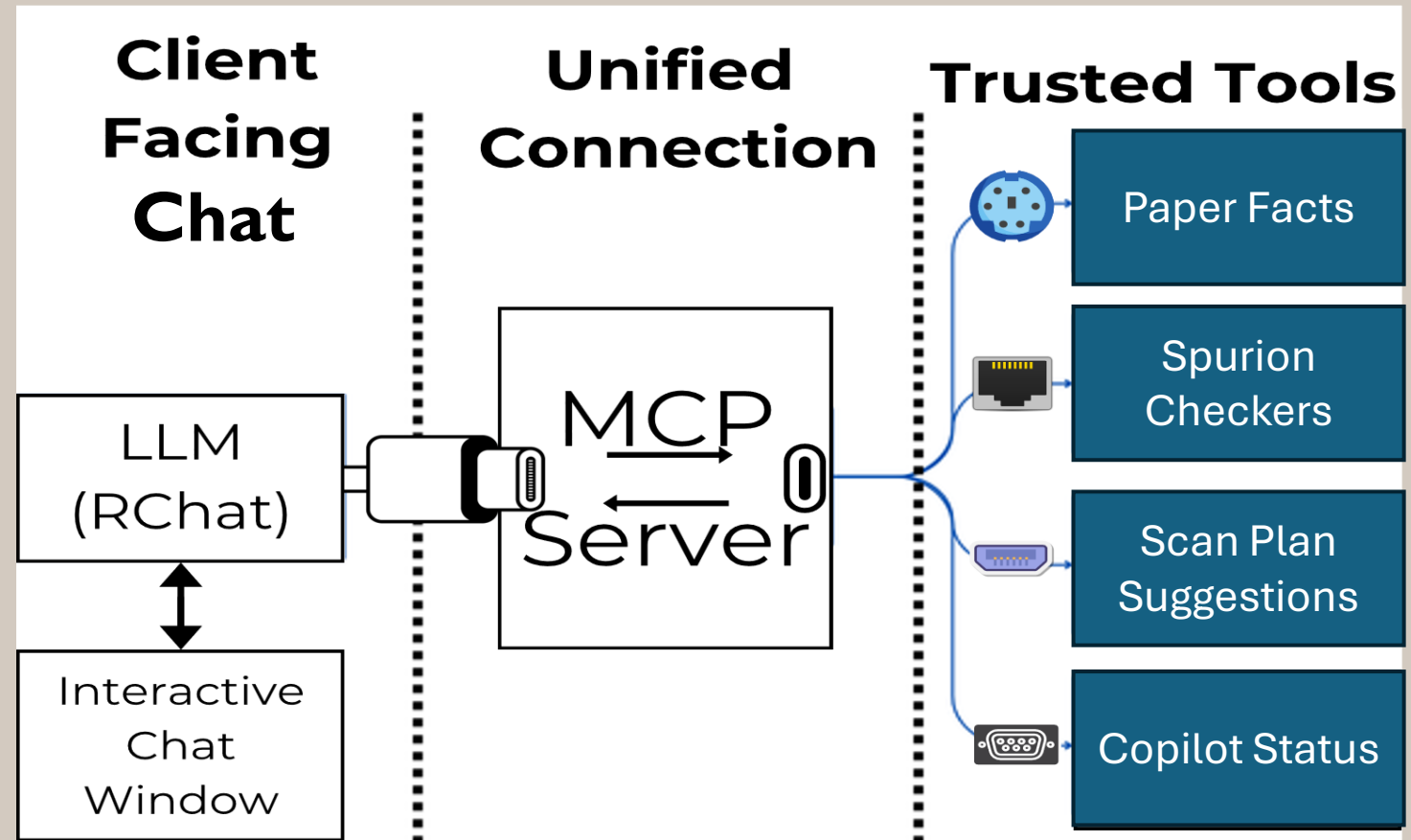
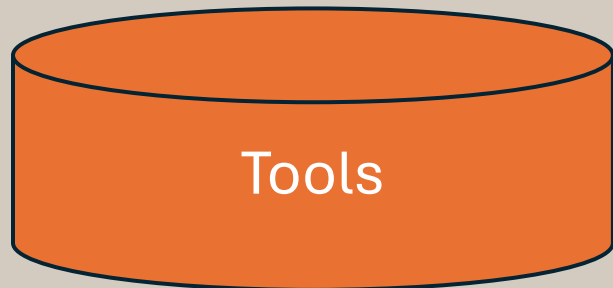
Chat UI + Models



Open Web-UI based
RChat models, currently

Model Context Protocol (MCP) – Tool Architecture

- Developed by Anthropic AI
- Way to access **trusted** tools
- I used this framework to connect NCNR tools to the LLM



Safety

Allows or Blocks

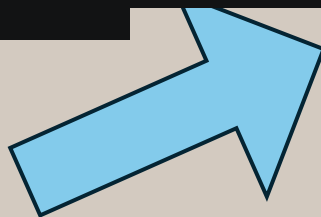
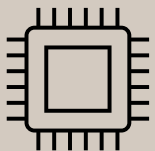
```
1 """MCP gateway over the bounded copilot router intents.
2
3 Phase 1 of the chat-interface plan (see HANDOFF.md, "Chat Interface / MCP
4 Gateway Plan"): expose the curated `copilot_ask` intents as MCP tools with
5 flat arguments, so any MCP client (Claude Code, a local-model chat shell)
6 can drive tascopilot through a typed, shell-free surface.
7
8 Design rules, in priority order:
9
10 - **"LLM proposes, registry disposes."** Every tool call goes through the
11 deterministic `copilot_ask` router with an explicit intent; the router
12 applies the live-control block to the question text, validates inputs,
13 and computes runnable/missing-input state. The gateway never executes
14 workflows itself.
15 - **Generated, not hand-written.** Tool names, descriptions, required
16 inputs, and example questions come from `COPILOT_INTENT_EXAMPLES` - the
17 same source that feeds the route-quality evals and the situational index
18 - so the MCP surface cannot drift from the router.
19 - **Flat arguments.** Local 27-70B models cannot reliably fill nested
```

9

```
10 - **"LLM proposes, registry disposes."** Every tool call goes through the
11 deterministic `copilot_ask` router with an explicit intent; the router
12 applies the live-control block to the question text, validates inputs,
```

```
35 requiring instrument-scientist review.
36 """
```

AI Proposes

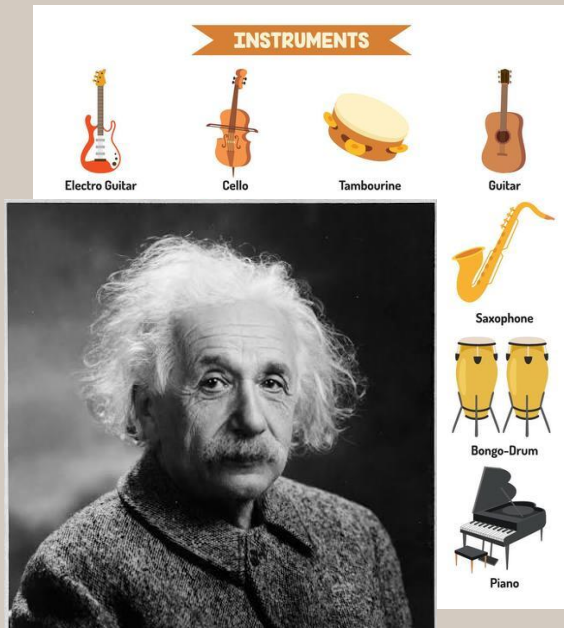


Instructions

Impact & Future – To Conclude – TL;DR



Who Benefits



Next Steps

- More tools
- Expand beyond BT-7
- Publish Paper



Bigger Vision
Other Facilities adopt
the co-pilot structure



Right Now!

- Available on tascopilot.ncnr.nist.gov!
- Ready for beta-testing with experiments
- In preparation for reactor start-up on August 19th



Acknowledgements:

Dr. William Ratcliff for guiding me throughout this process

Dr. Julie Borchers for helping with all the administrative processes

CORE Program for giving me the opportunity learn from my mentor

NSF for supporting CHRNS

Parents for supporting me

Fellow SURF and CORE students!

Thank you to all who made this possible!

Thank you!

Questions?