Applications of Large Language Models and AI to Neutron Scattering

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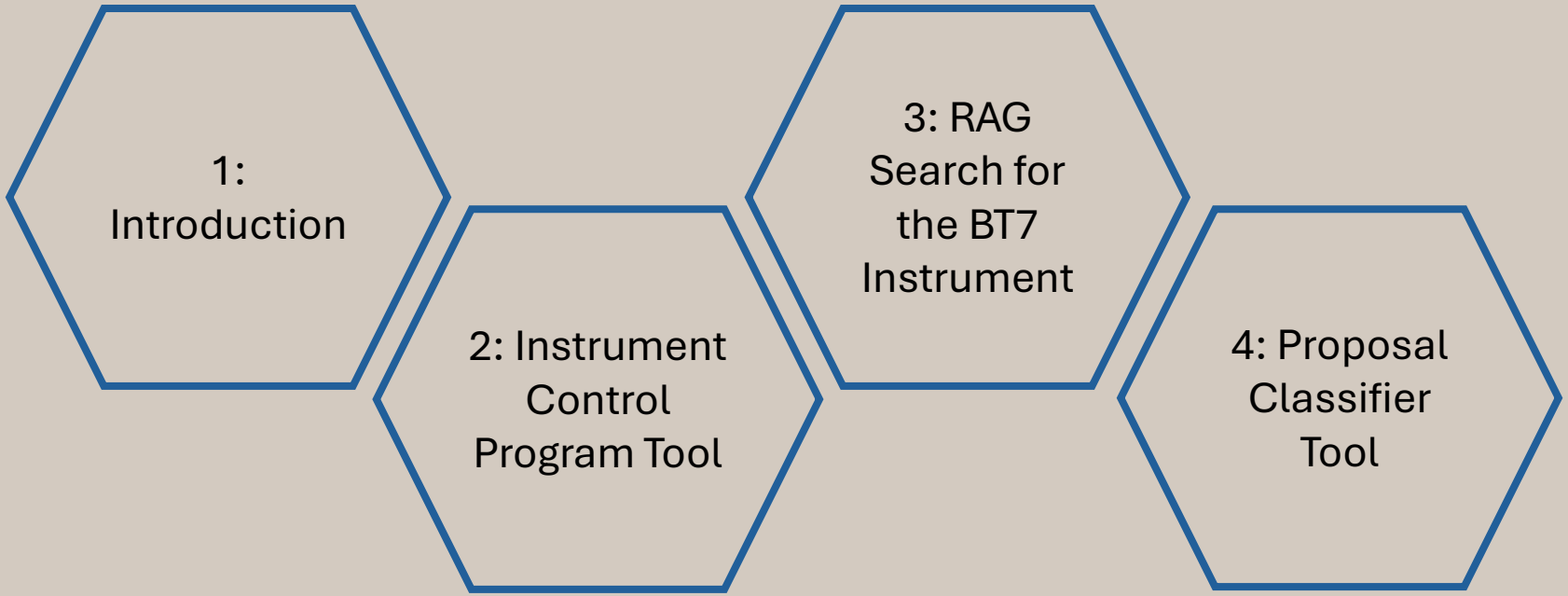
National Institutes of Standards and Technology
Center for Neutron Research

Table of Contents



1: Introduction

Background – The NCNR

- User facility
- Limited beam time

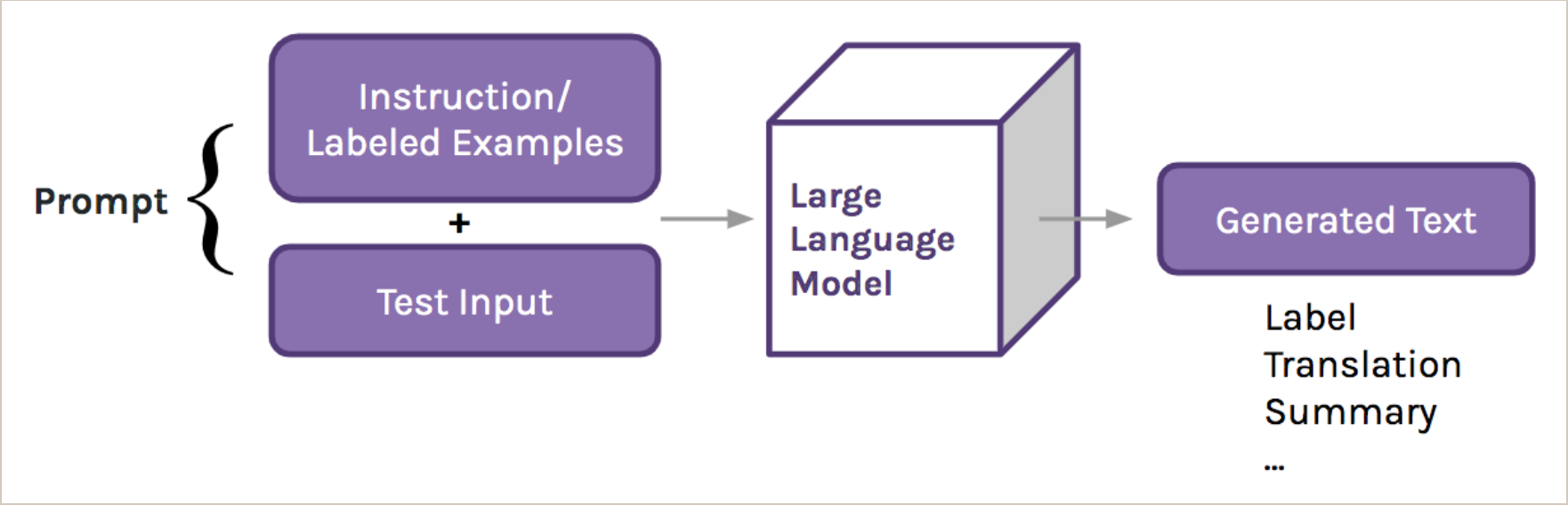
Abstract – Main Ideas

How can large language models (LLMs) help the NCNR?

- Sort Documents
- Calculate values
- Search for relevant information

What is a Large Language Model (LLM)?

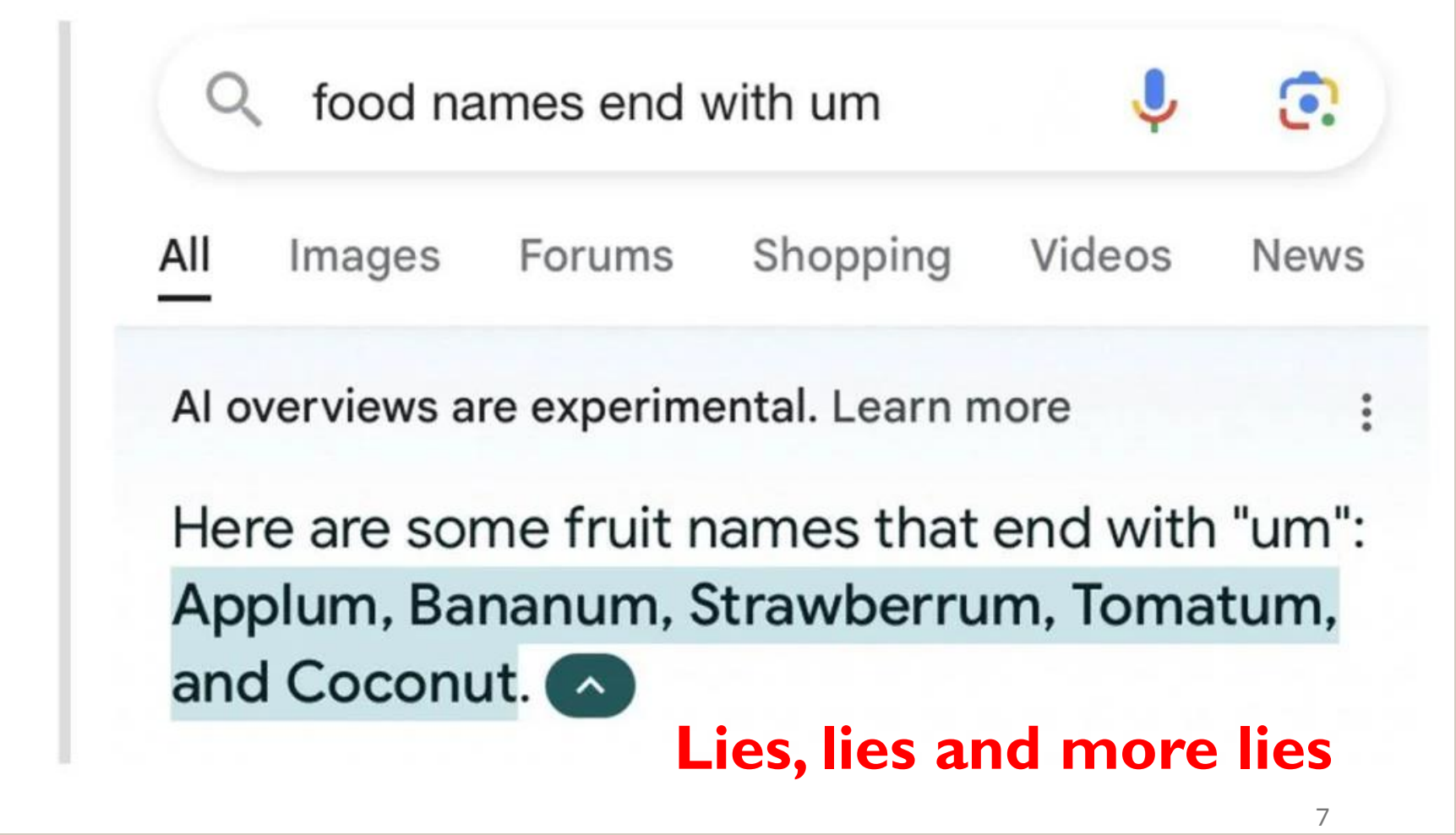
- Trained on large text datasets to learn language patterns.
- Predicts the next word based on context.
- Produces fluent, relevant language outputs.



Blevins, T. (2023, July 9). *What do LLMs know about linguistics? It depends on how you ask*. The Gradient. Retrieved from https://thegradient.pub/what-do-llms-know-about-linguistics-it-depends-on-how-you-ask/

Problem

- LLMs can hallucinate



Abstract

How can large language models (LLMs) help the NCNR?

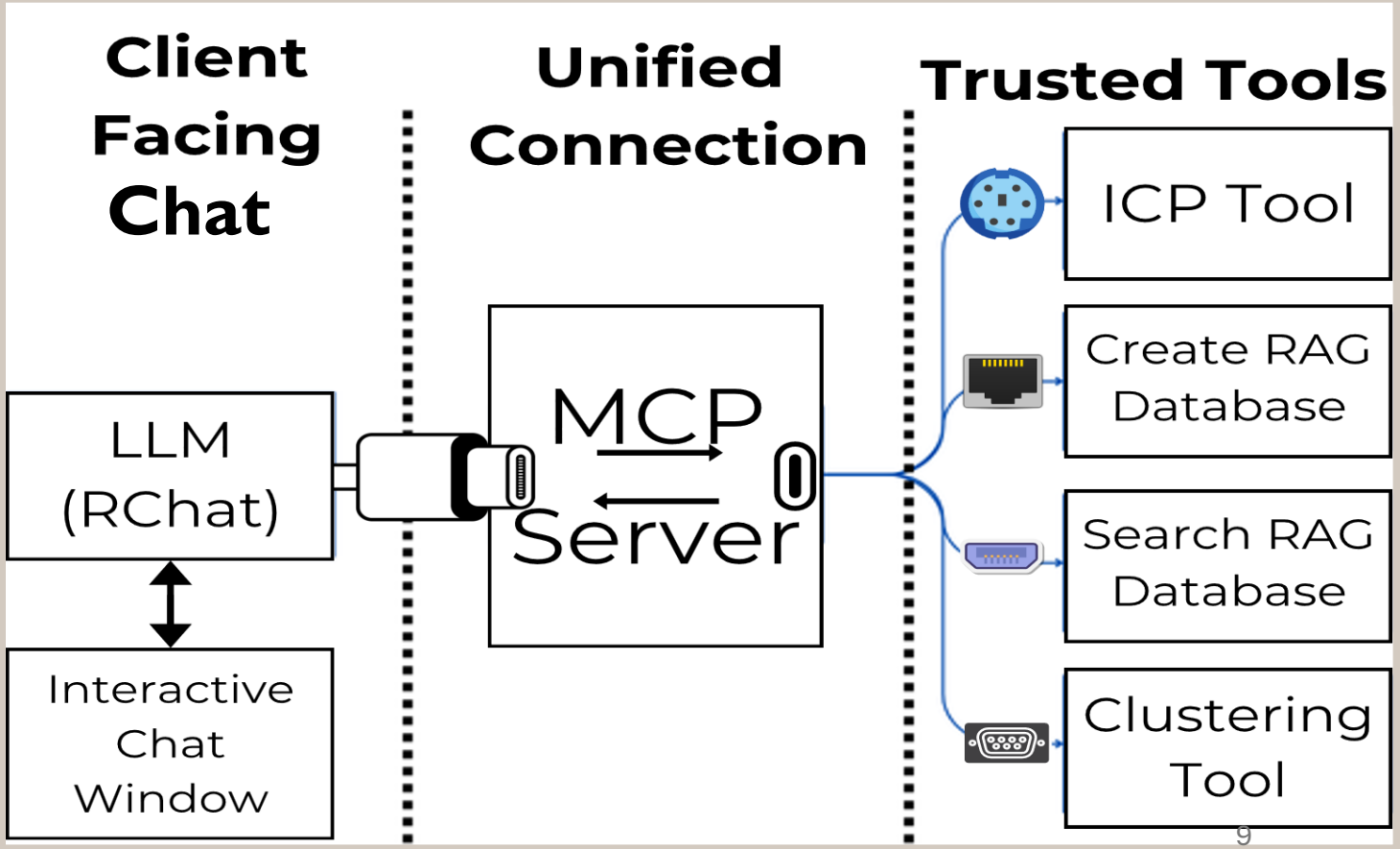
- Sort documents
- Calculate values
- Search for relevant information

How can we fix LLMs to not hallucinate while doing this?

Answer:

Give it Trusted Tools – Model Context Protocol

- Developed by Anthropic AI
- Way to access **trusted** tools
- "Unifying APIs"
- Adaptive Tool Access



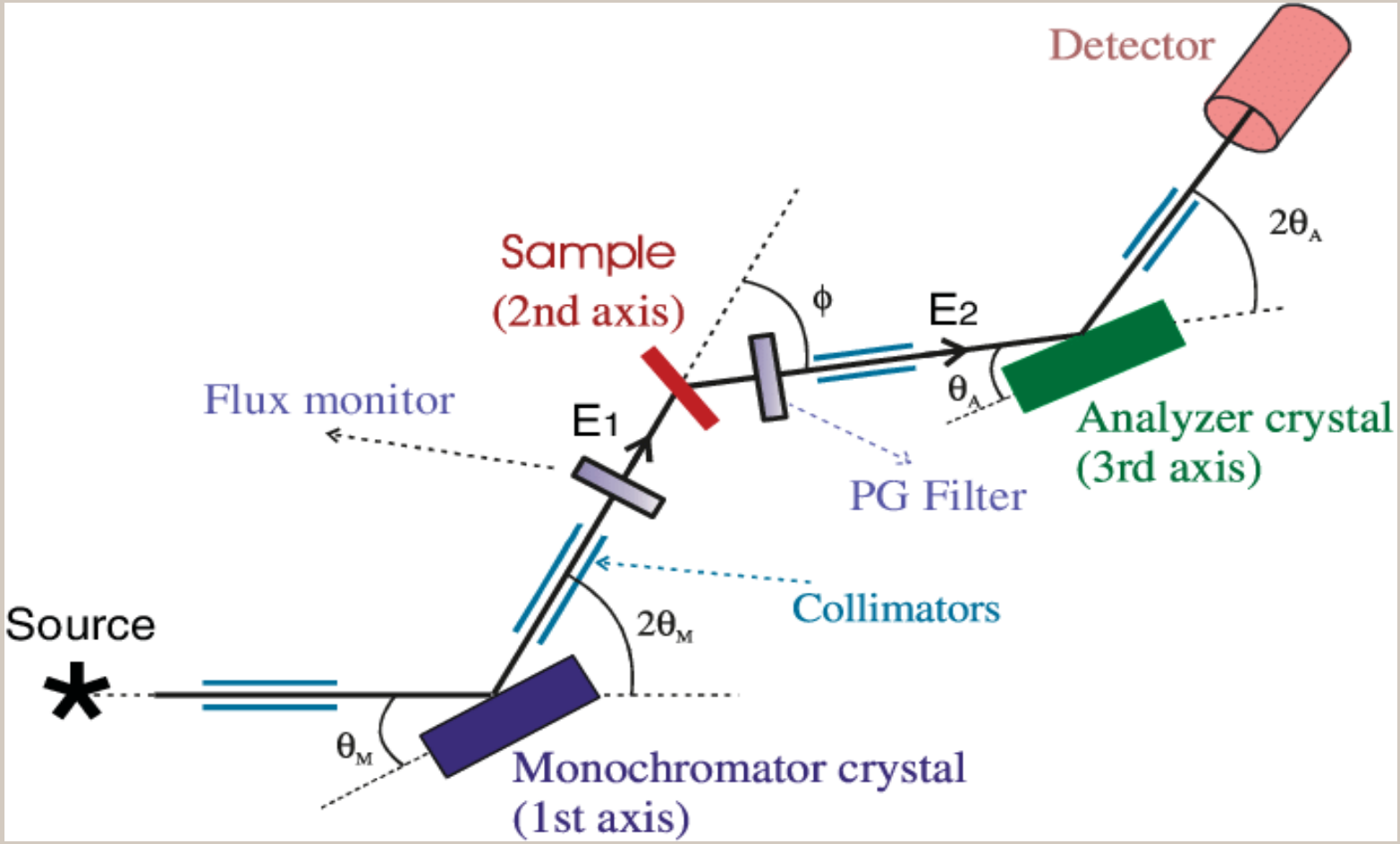
Tools to Help Users

Instrument Control Program (ICP) Tool

For the BT7 Instrument

The Problem to Solve

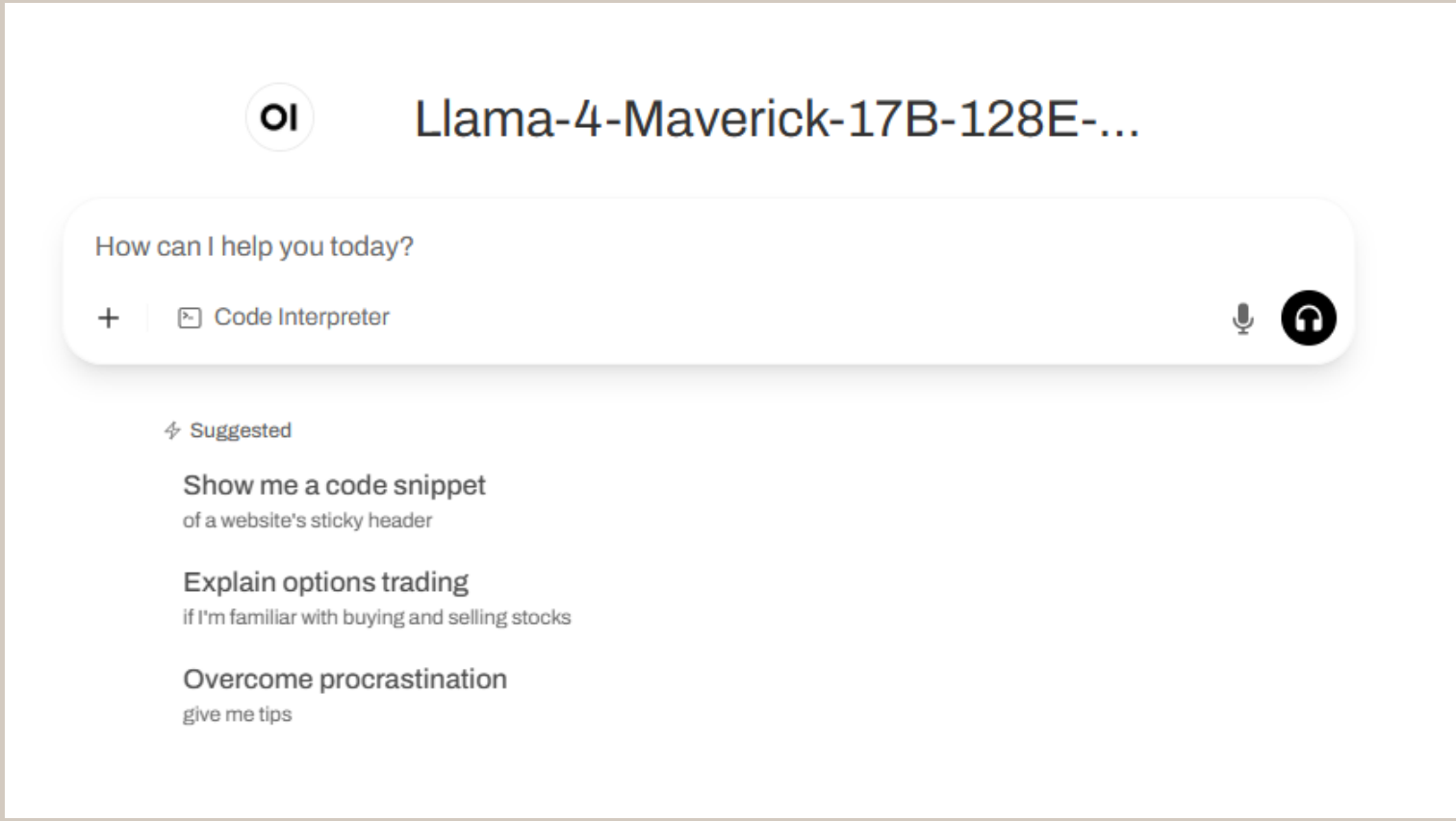
- Users want to plan their experiment and to perform motor calculations when not at the instrument



Li, G., Bentoumi, G., Tun, Z., Li, L., & Sur, B. (2016, July 26). Thermal neutron scattering cross-section measurements of heavy water. *CNL Nuclear Review*, 1–7. https://doi.org/10.12943/CNR.2016.00008

The Solution – ICP tool

- Computes motor angles
- Based on standalone trusted python script
- Allows for Natural Language input (LLM)



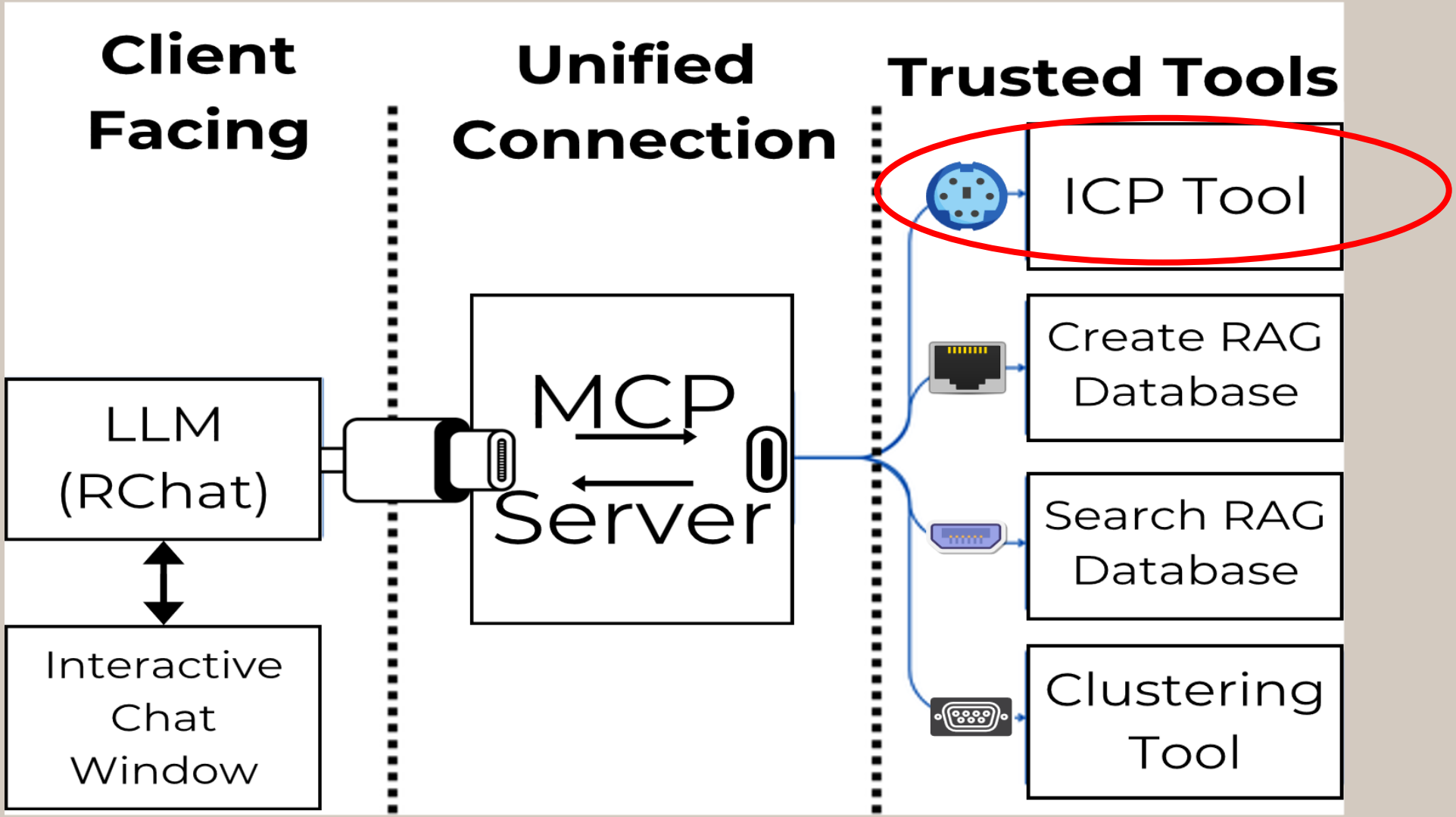
Steps to do this

- Get input from LLM
- Get output from tool
- Give back to chat interface

What will do this

- **Model Context Protocol**

Model Context Protocol

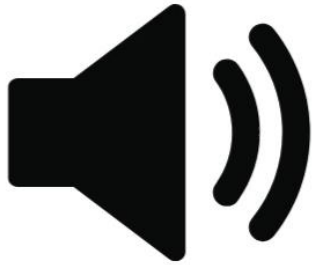


Video Demo

Instrument Control Program

Tool Demonstration

By: Aditya Purohit



Retrieval Augmented Generation Search for the BT7 Instrument

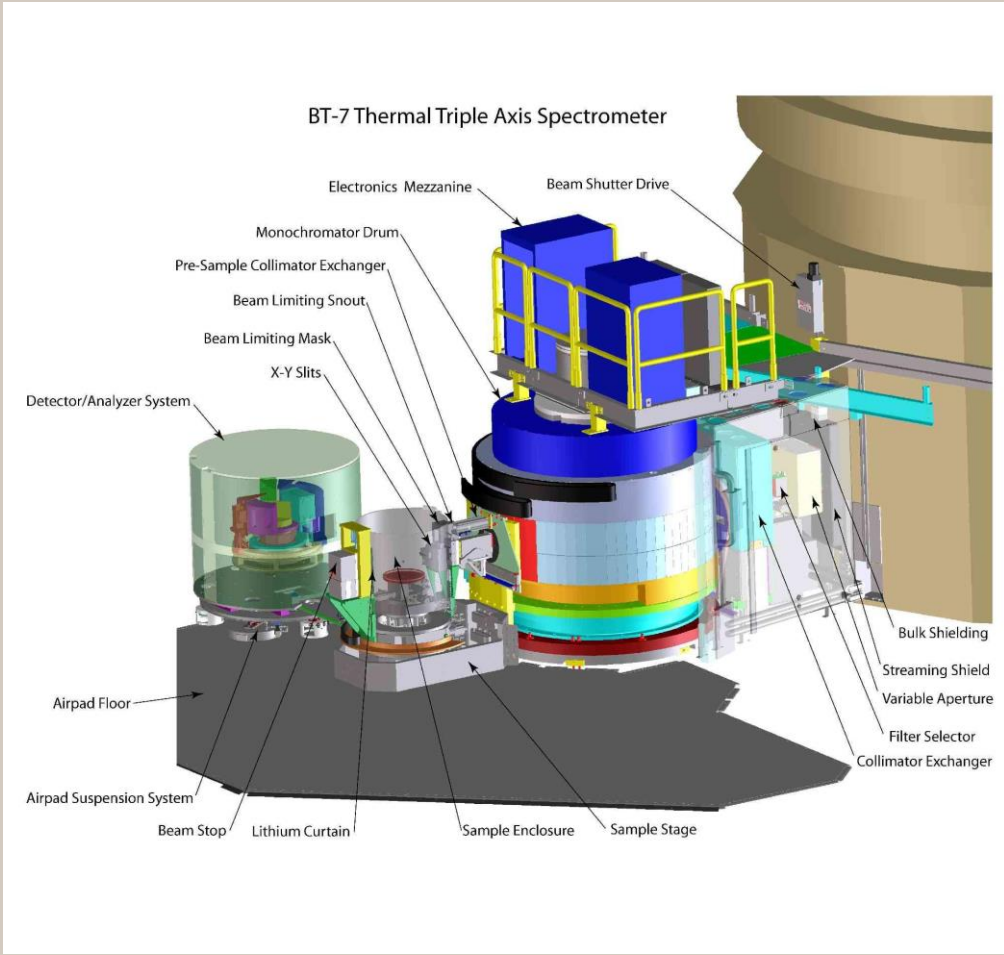
The Problem to Solve

- Takes time to search through documents
- Having information from papers published using the instrument can help answer user questions

(n.d.). *Late-night paperwork sorting* [Stock photo]. StockCake. Retrieved from https://stockcake.com/i/late-night-paperwork-sorting_1390566_917312

The Solution – RAG on BT7 Papers

- Allows users to quickly search documents through a chat interface
- Pulling from papers given to it, for accuracy
- Allow for the user to read the papers used for response

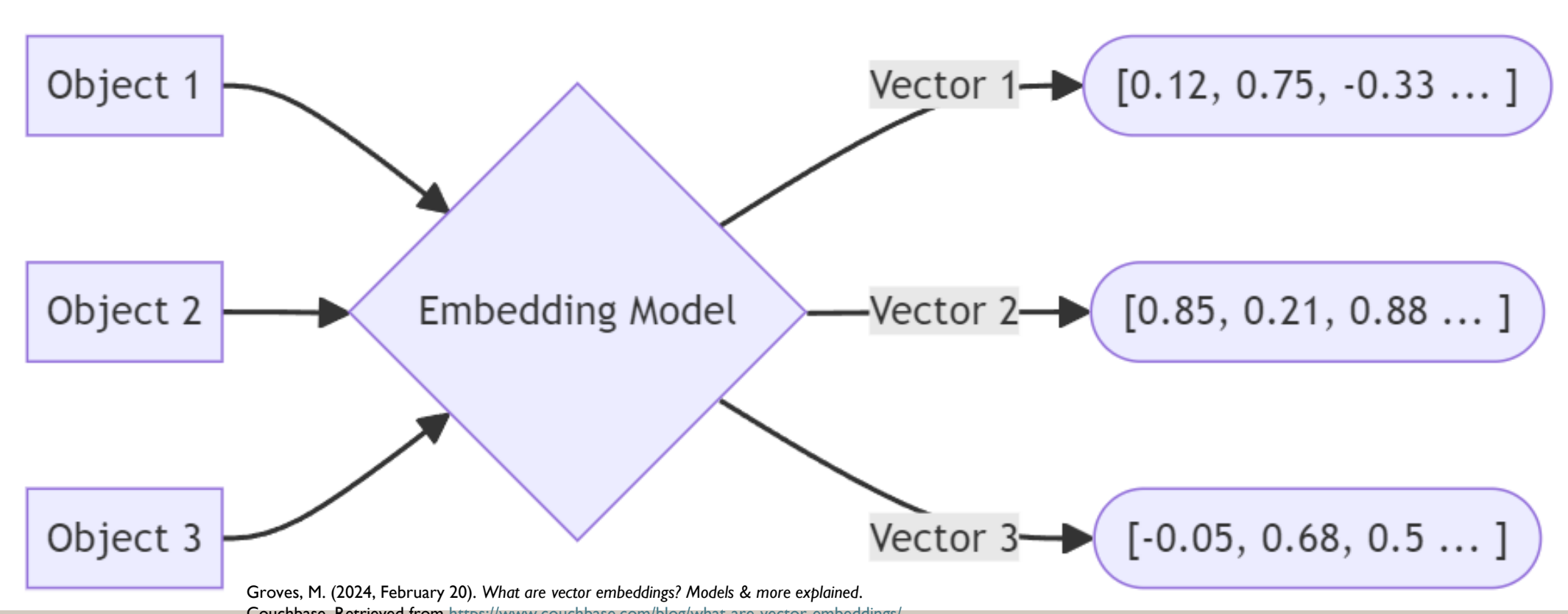


National Institute of Standards and Technology. (2018, December 19). *BT-7 double-focusing triple-axis spectrometer*. NIST Center for Neutron Research. Retrieved from https://www.nist.gov/ncnr/bt-7-double-focusing-triple-axis-spectrometer

Steps to do this	What will do this
Intake documents	Model Context Protocol
Input query from LLM	MCP
Embed to vector database/graph	Embedding Model

What is an Embedding Model?

- Used to convert text to vectors

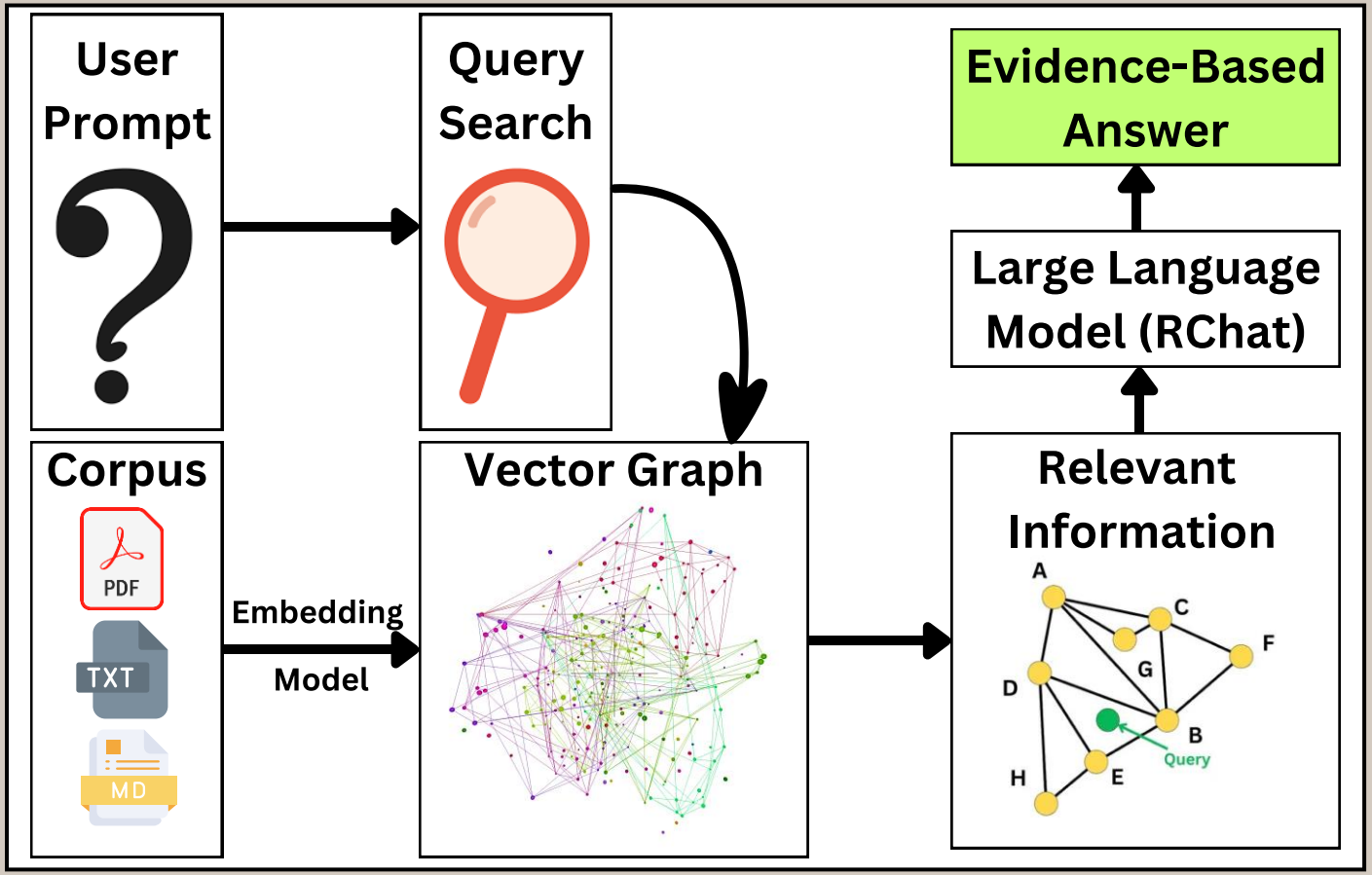


Groves, M. (2024, February 20). *What are vector embeddings? Models & more explained.* Couchbase. Retrieved from https://www.couchbase.com/blog/what-are-vector-embeddings/

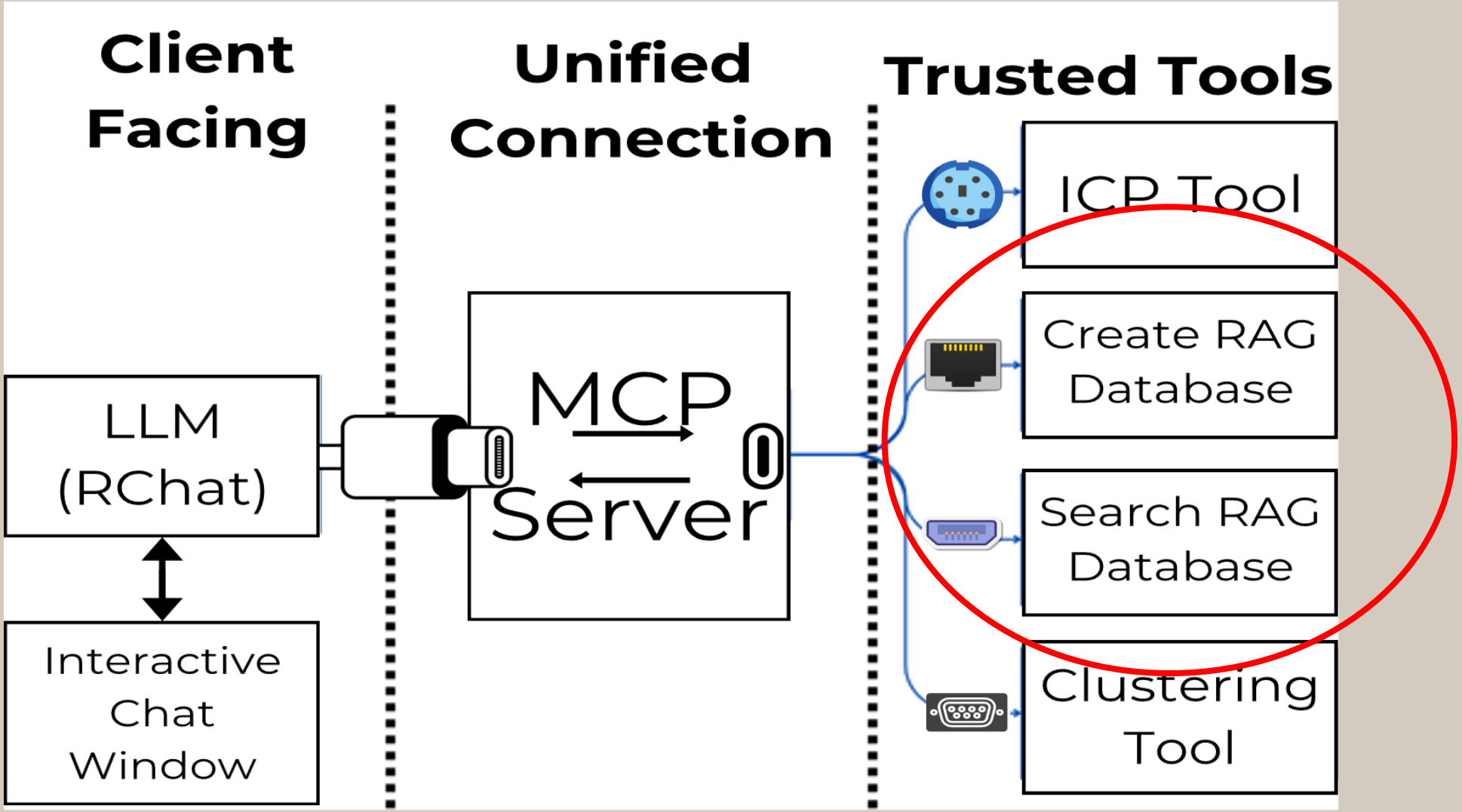
Steps to do this	What will do this
Intake documents	Model Context Protocol
Embed to vector database/graph	MCP
Input query from LLM	Embedding Model
Retrieve relevant information	RAG

What is Retrieval Augmented Generation (RAG)?

- Enables Accurate Searching
- Will only search given docs
- Reduces Hallucinations
- Allows for backchecking



Steps to do this	What will do this
Intake documents	Model Context Protocol
Input query from LLM	Embedding Model
Embed to vector database/graph	MCP
Retrieve relevant information	RAG
Give to LLM to craft answer	MCP


Client Facing
Unified Connection
Trusted Tools
LLM (RChat)
Interactive Chat Window
MCP Server
ICP Tool
Create RAG Database
Search RAG Database
Clustering Tool

Steps to do this	What will do this
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Video Demo

BT7 Retrieval Augmented Generation Tool Demonstration

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NCNR Proposal Classifier

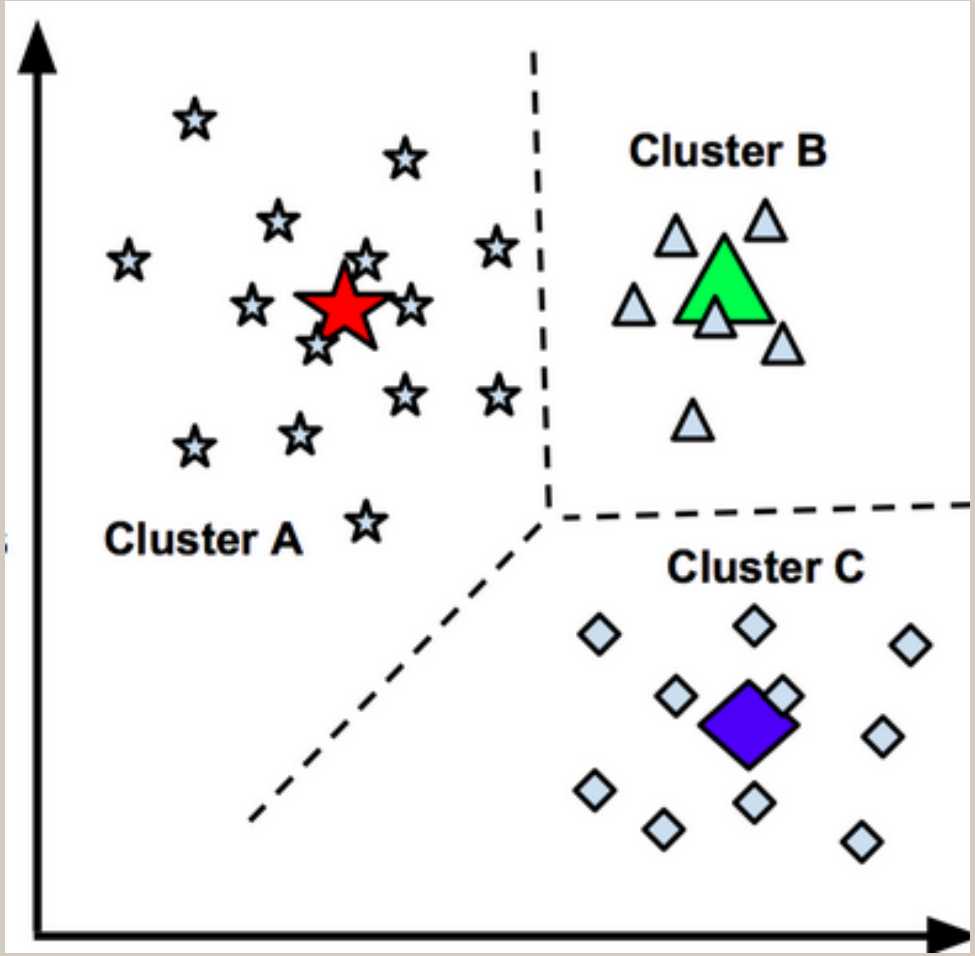
The Problem to Solve

- NCNR Proposal Call contains 500+ proposals
- One person sorts these by area of expertise to send to reviewers
- Proposals are only grouped, NOT reviewed

(2016, December 25). *Piles of paper stacked neatly on table* [Stock photo]. Shutterstock. Retrieved from https://www.shutterstock.com/image-photo/piles-paper-stacked-neatly-on-table-542487283

The Solution – Proposal Classifier Tool

- Group the documents
- Give top 5 keywords for each group
- Send clusters to respective reviewers

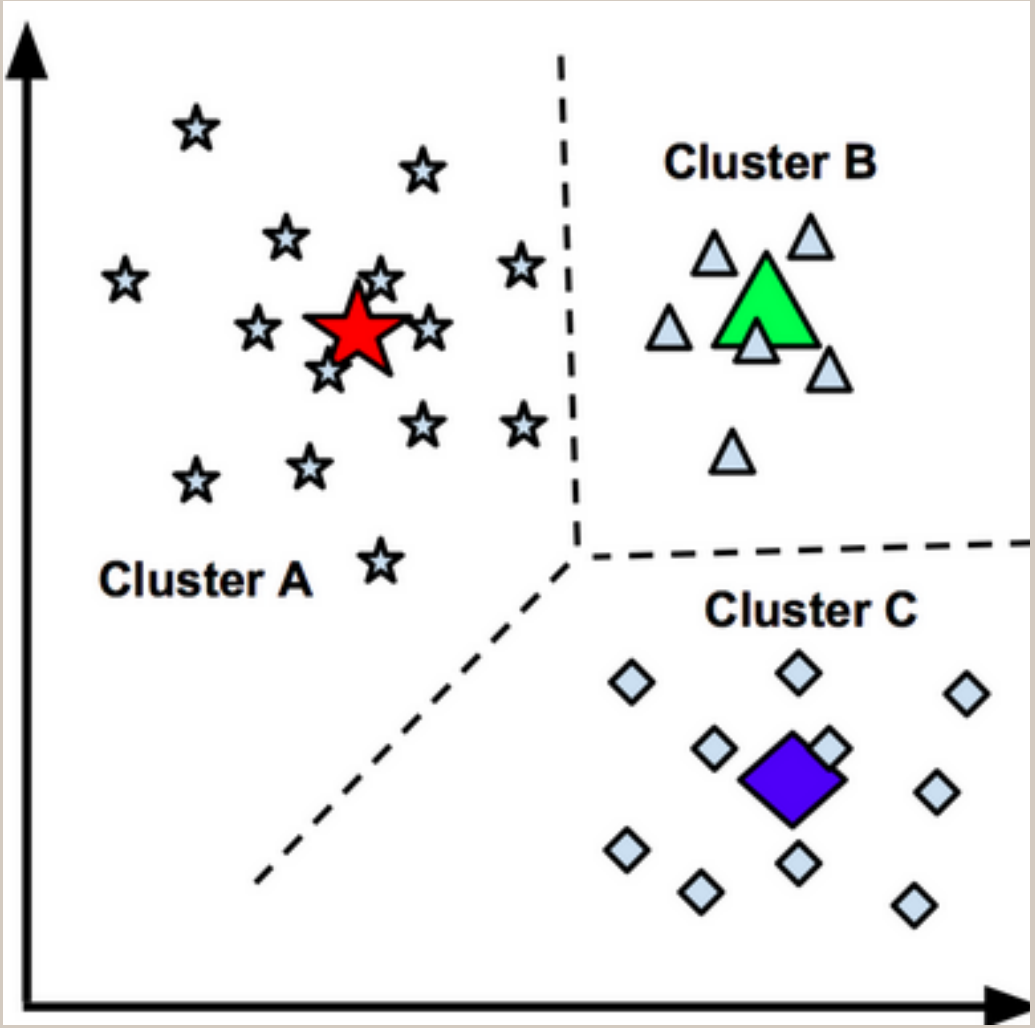


Dasila, M. S. (2019, May 1). *Basics: K-means clustering algorithm*. Medium. Retrieved from https://medium.com/@msdasila90/basics-k-means-clustering-algorithm-a77c539c9e00

Steps to do this	What will do this
Text to vectors	Embedding Model
Compare then group vectors	Clustering Algorithm

What is Clustering?

- Unsupervised Learning
- Groups similar data based on features
- KMeans Clustering – Distance between documents, and means the distance



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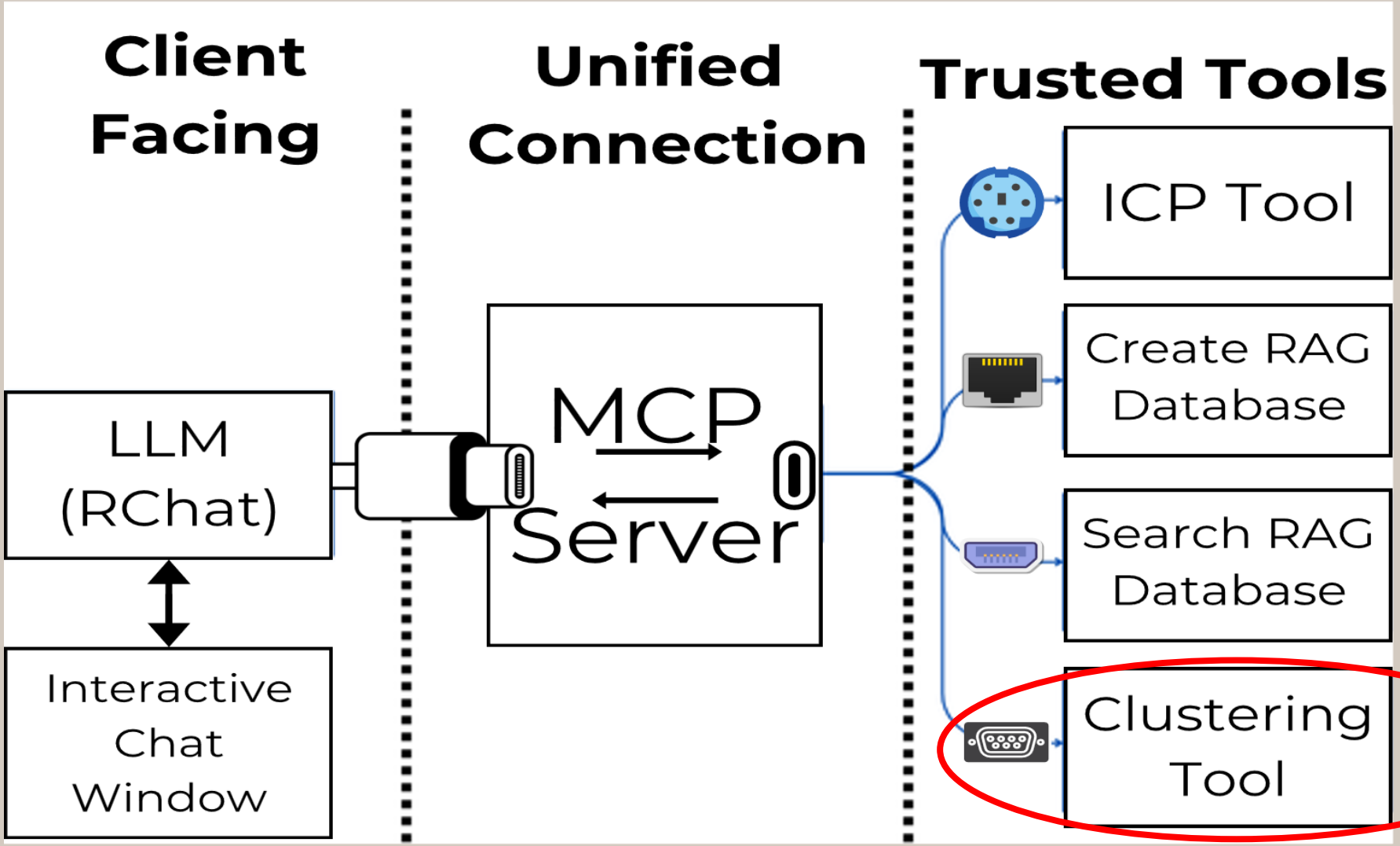
Steps to do this	What will do this
Text to vectors	Embedding Model
Compare then group vectors	Clustering Algorithm
Give Keywords for Groups	RAG
Give back to the user	MCP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Video Demo

NCNR Proposal Classifier Tool

By: Aditya Purohit

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NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

CHRNS
CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING

Thank you!

Questions?