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

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

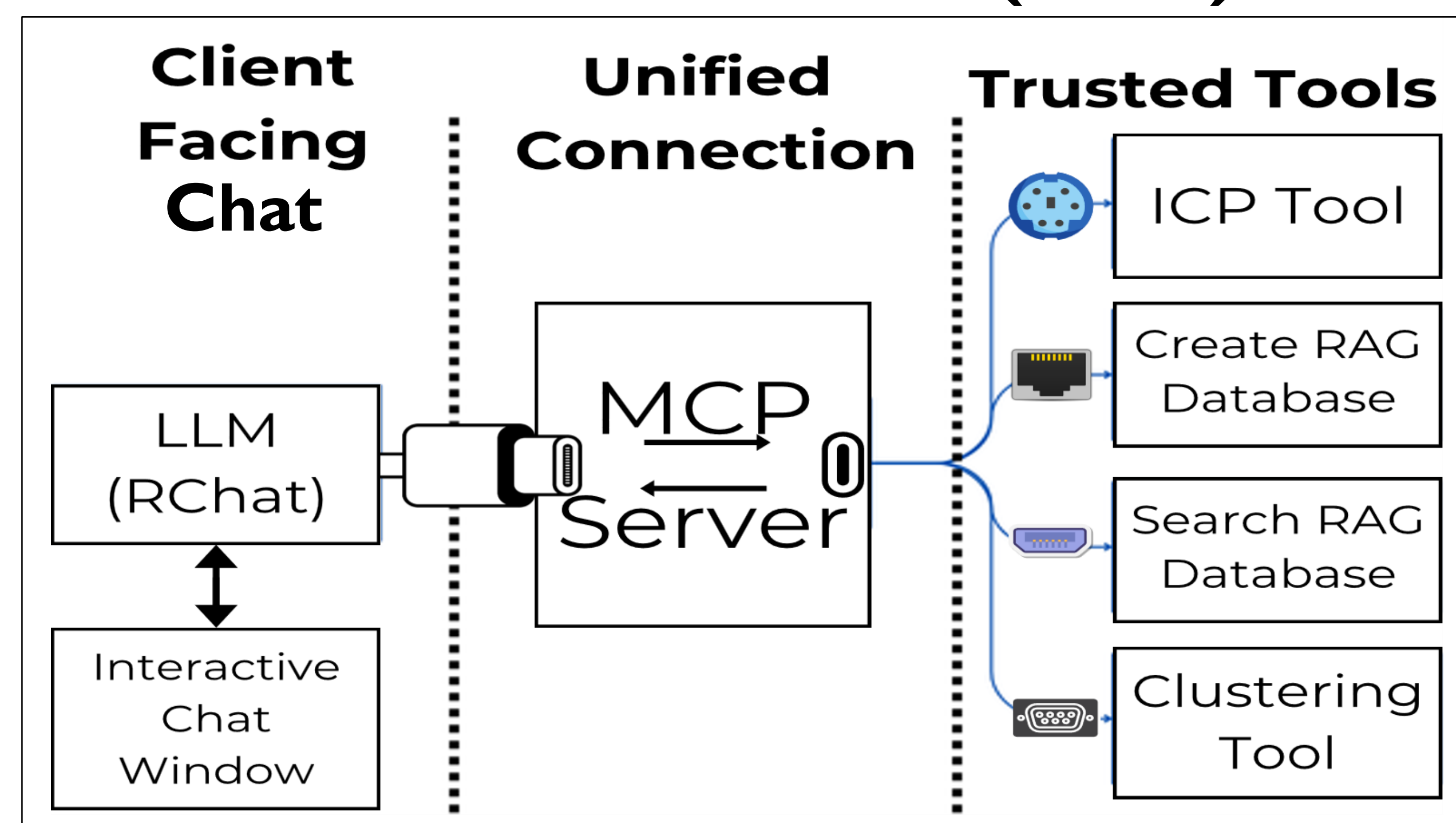CHRNS — Center for High Resolution Neutron Scattering

Video Demos:

Abstract & Methodology

This project explores the integration of large language models (LLMs) to enhance neutron scattering and research workflows at the NIST Center for Neutron Research (NCNR). As a user facility, the NCNR serves many researchers who may not have deep familiarity with each instrument's capabilities or relevant prior work. By leveraging the Model Context Protocol (MCP), LLMs can access accurate, validated tools and data sources. Key components include an Instrument Control Program (ICP) tool that translates motor positions into physical coordinates via a chat interface, and a Retrieval-Augmented Generation (RAG) system that enables fast, targeted searches across NCNR publications. Additional efforts include integrating AI for document classification and semantic search to streamline the proposal review process. These tools collectively help users better understand instruments, speed up scientific preparation, and support more efficient research at the NCNR.

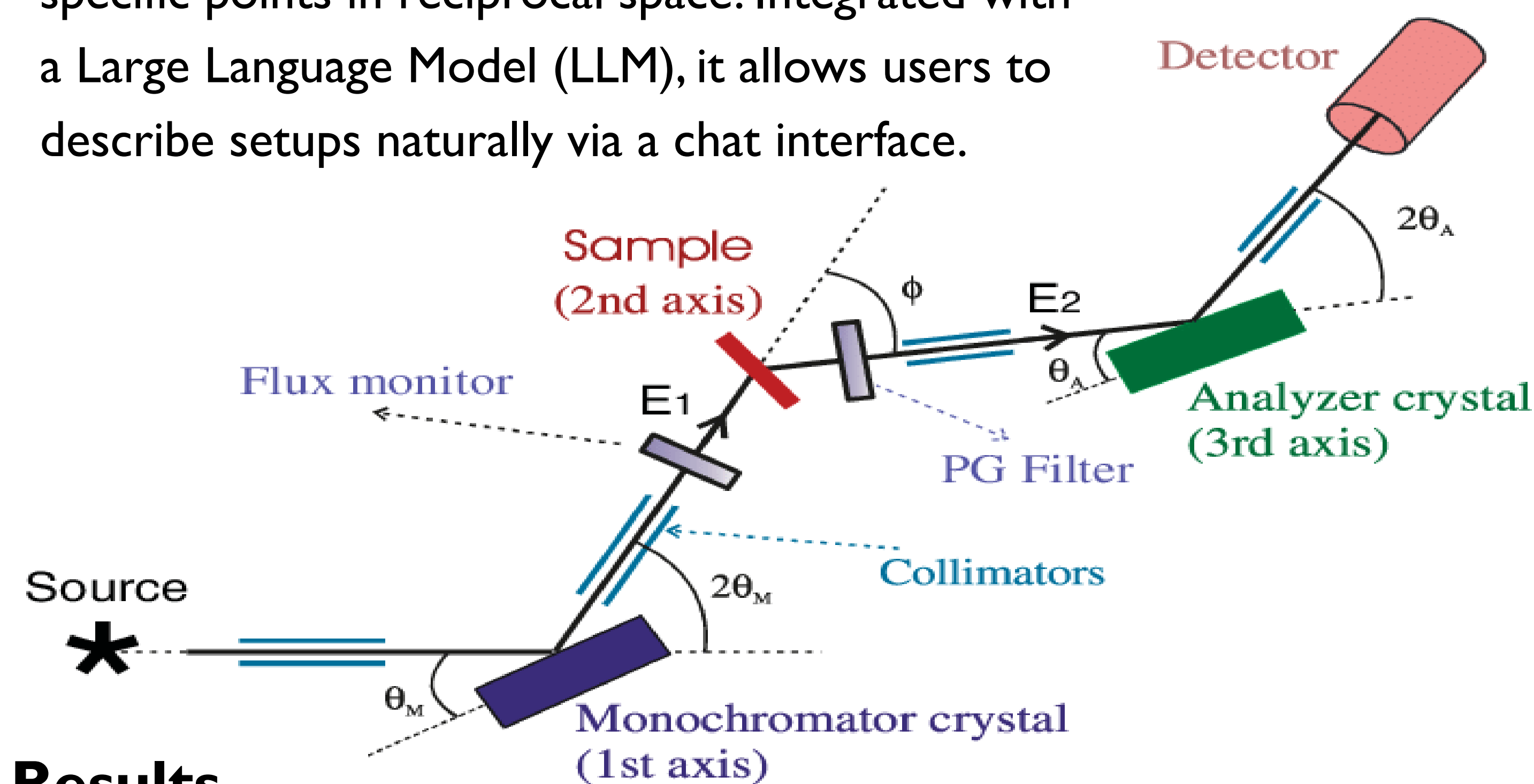## LLM Tool Interface (MCP)

Client Facing Chat — LLM (RChat) — Interactive Chat Window

Unified Connection — MCP Server

Trusted Tools — ICP Tool, Create RAG Database, Search RAG Database, Clustering Tool

Instrument Control Program Tool

Tool Description

The Instrument Control Program (ICP) tool computes motor angles for triple-axis spectrometers based on crystallographic inputs, targeting specific points in reciprocal space. Integrated with a Large Language Model (LLM), it allows users to describe setups naturally via a chat interface.
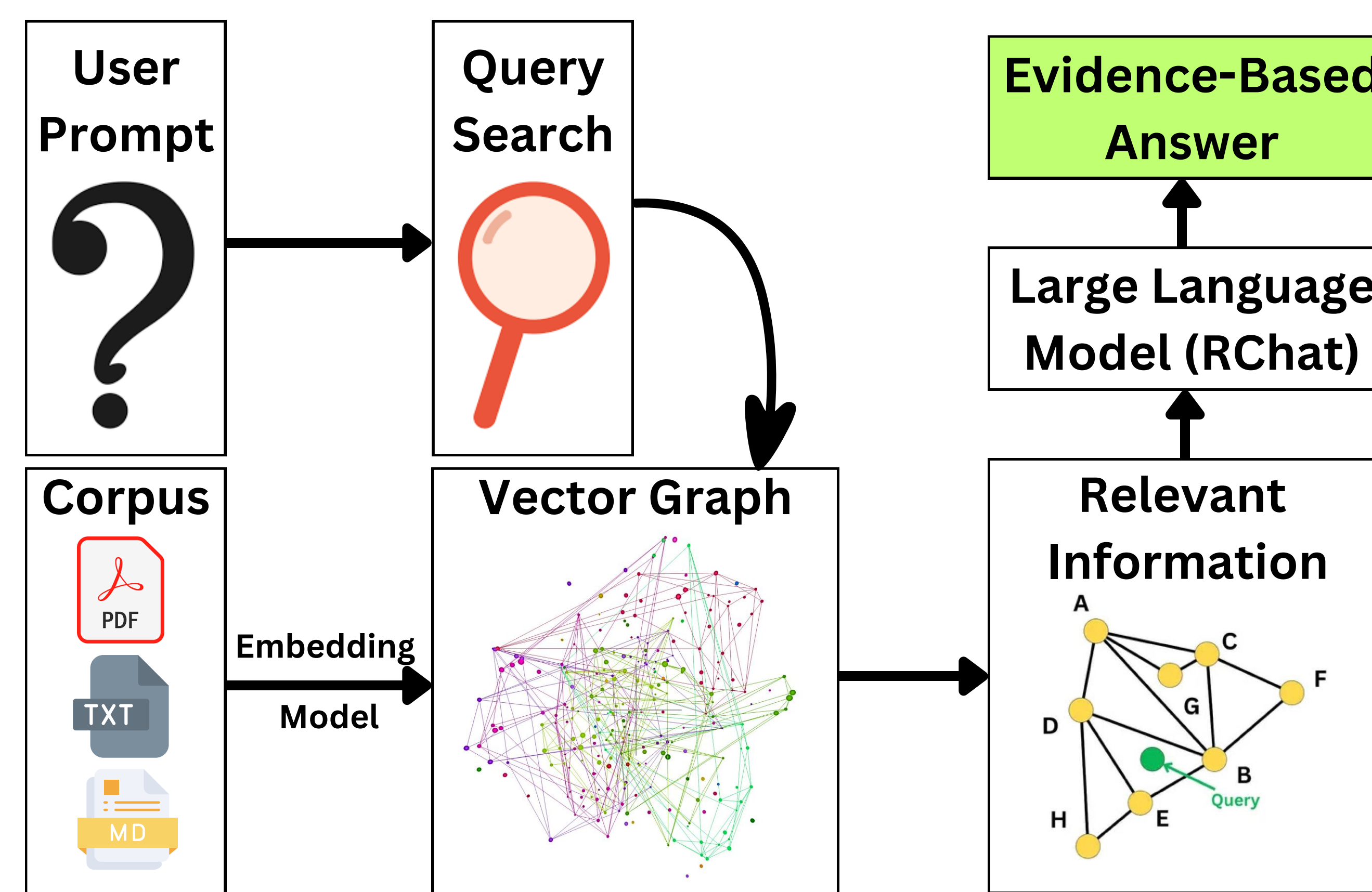

Detector; Sample (2nd axis); E_2; $2\theta_A$; Analyzer crystal (3rd axis); ϕ; PG Filter; Flux monitor; E_1; Collimators; Source; $2\theta_M$; θ_M; Monochromator crystal (1st axis)

Results

✓ Reduces setup complexity
✓ Speeds up configuration and increases efficiency
✓ Makes tool more accessible to non-expert users in experimentation

Future Directions

• Integration with other tools to allow for a seamless workflow

Retrieval Augmented Generation (RAG) for BT7 Instrument

User Prompt → Query Search → Evidence-Based Answer

Corpus (PDF, TXT, MD) → Embedding Model → Vector Graph → Relevant Information → Large Language Model (RChat)

BT7 RAG Tool

The BT7 RAG tool uses a database of NCNR papers from 2016–17 to help researchers quickly reference relevant experimental setups, parameters, and results. By linking natural language queries to past BT7 studies, it streamlines experiment planning and enhances understanding of the instrument's capabilities.

Results

✓ More efficient literature search
✓ Increases the accuracy of outputs
✓ Chat interface that creates a coherent response from the data

Future Directions

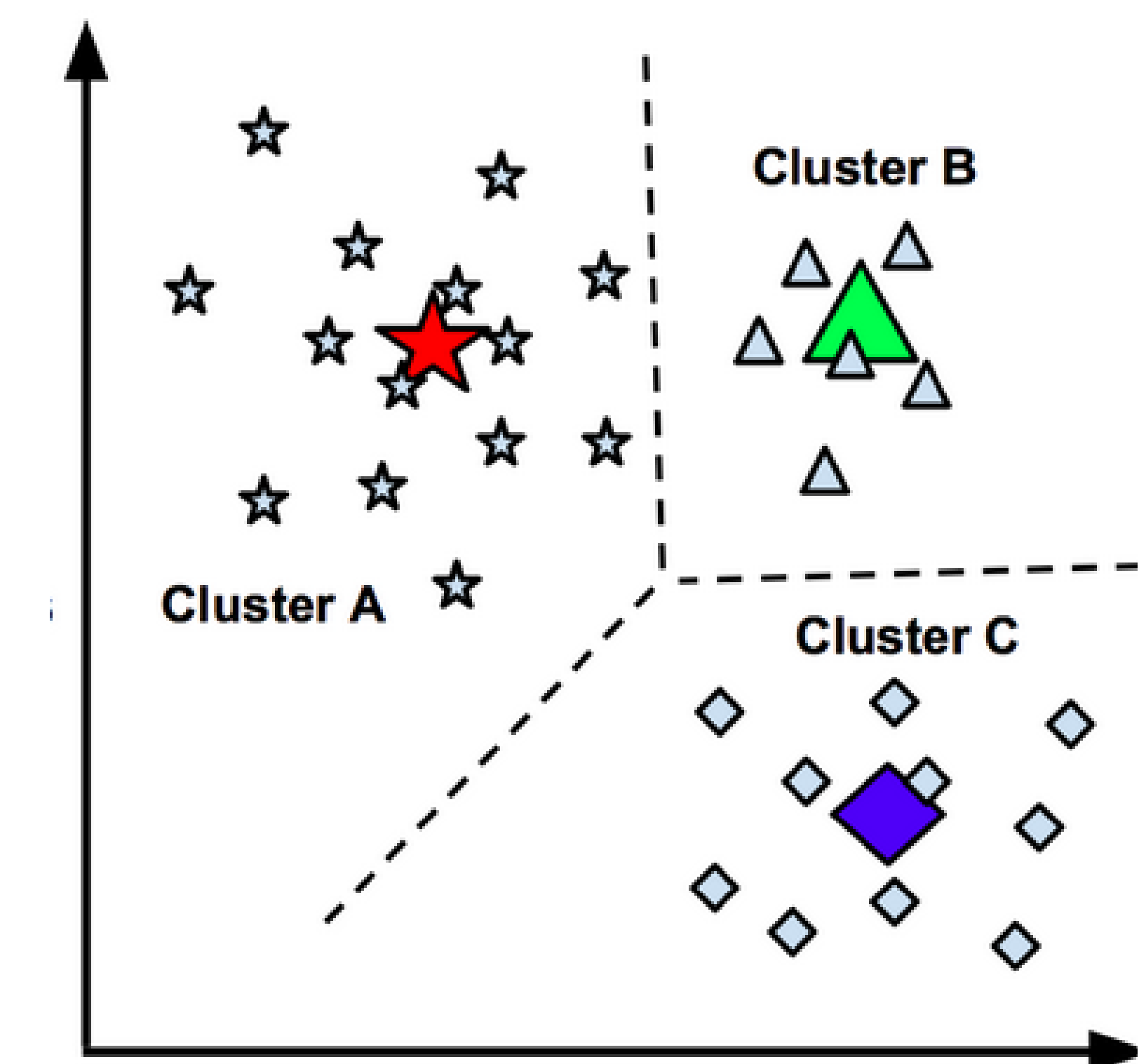• Customize to add the documents of different instruments and/or labs

Proposal Classifier Tool

Clustering Background

Clustering groups similar data without labels to find natural patterns.

Cluster A; Cluster B; Cluster C

Tool Description

The Proposal Classifier tool uses semantic search and RAG-based clustering to organize incoming NCNR proposals by scientific themes. This aids staff in streamlining the review process, highlighting overlaps, and surfacing relevant prior work to support more informed evaluation.

Results

✓ Creates clusters and keywords to describe them
✓ Inputs and outputs through file path, no transferring required
✓ Allows for iteration to make focused proposal packages

Future Directions

• Add reviewers to keywords and have auto-assignment packages

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