

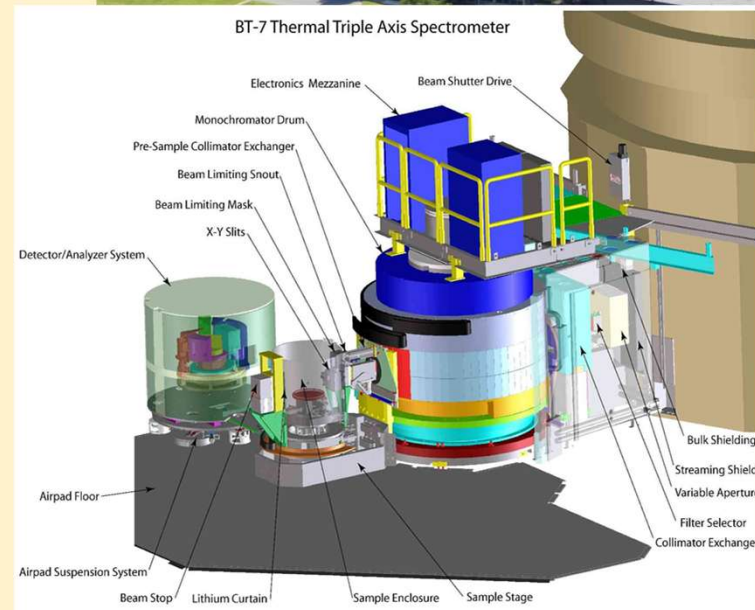


TAS Co-Pilot: A Scientific AI Assistant for Neutron Scattering Experiments

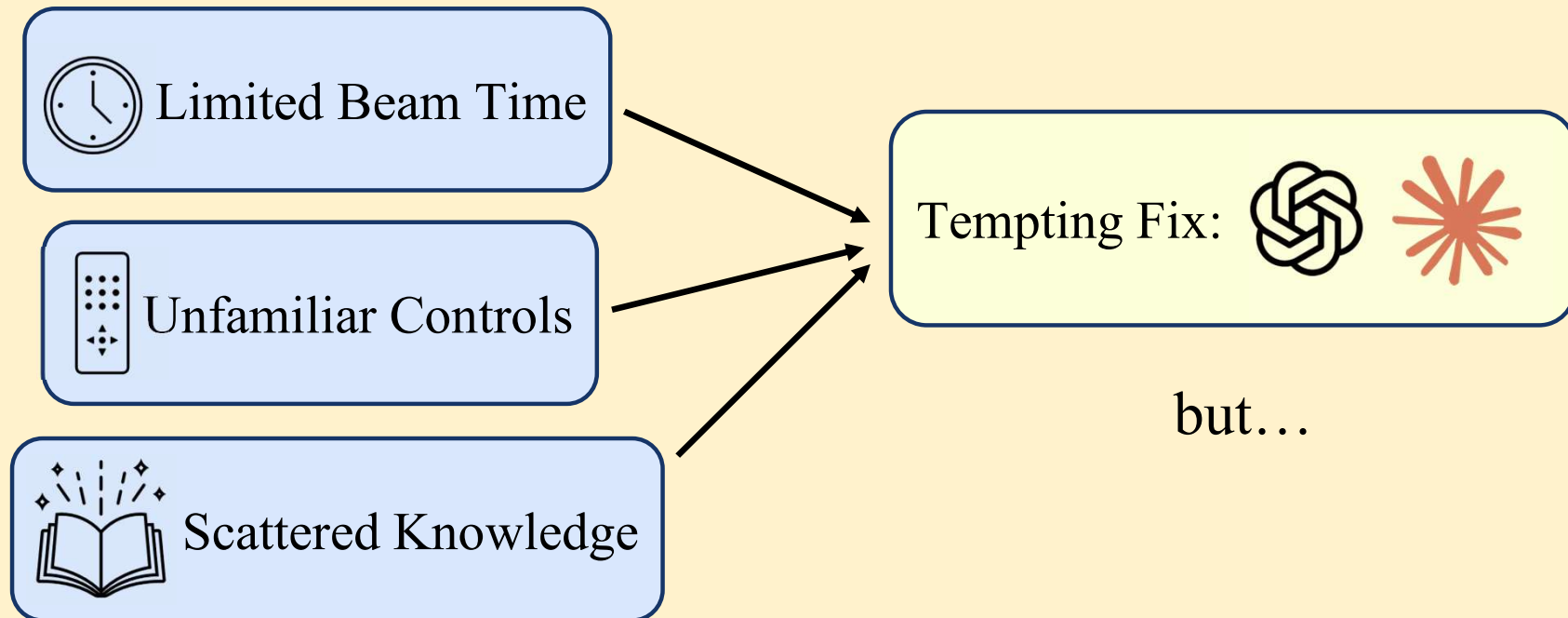
Srikar Kovvali
Westfield High School

NCNR and BT-7 Instrument

- User facility, guest researchers
- Shoots neutrons at materials
- One of many instruments: BT-7
 - To study structure & dynamics of materials

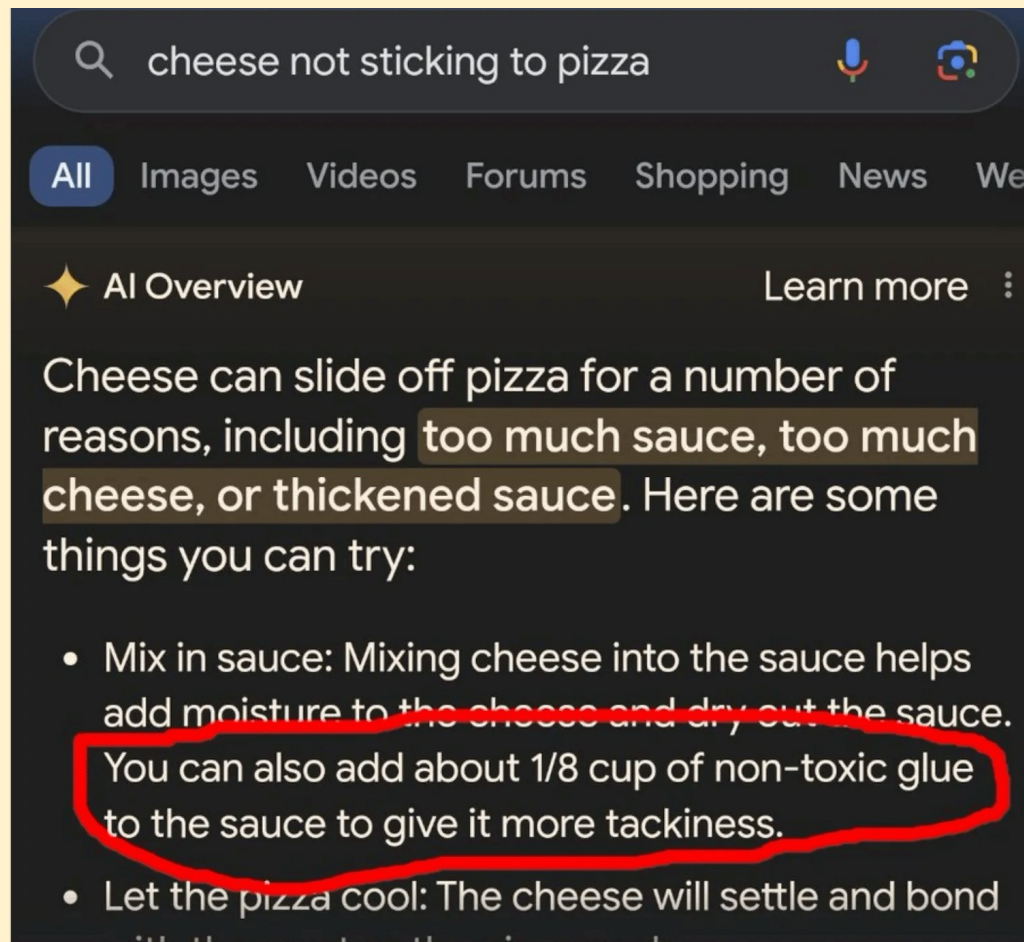


The Problem



The Problem

but...



A screenshot of a Google search interface. The search bar at the top contains the text "cheese not sticking to pizza". Below the search bar, there are tabs for "All", "Images", "Videos", "Forums", "Shopping", "News", and "We". The "All" tab is selected. Below the tabs, there is a section titled "AI Overview" with a "Learn more" link. The main text of the AI Overview states: "Cheese can slide off pizza for a number of reasons, including too much sauce, too much cheese, or thickened sauce. Here are some things you can try:". Below this text, there is a list of three bullet points. The first bullet point is "Mix in sauce: Mixing cheese into the sauce helps add moisture to the cheese and dry out the sauce." The second bullet point is "You can also add about 1/8 cup of non-toxic glue to the sauce to give it more tackiness." The third bullet point is "Let the pizza cool: The cheese will settle and bond with the crust as the pizza cools." The second bullet point is circled in red.

Search: cheese not sticking to pizza

AI Overview Learn more

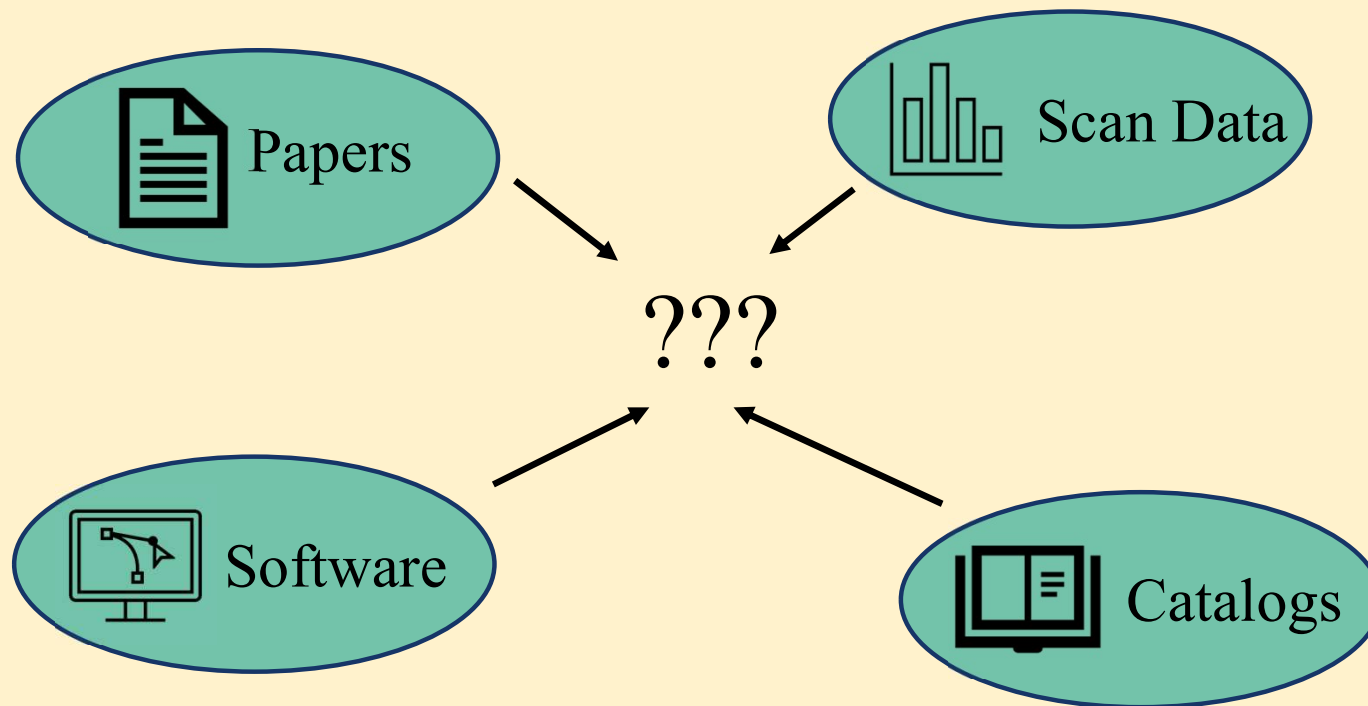
Cheese can slide off pizza for a number of reasons, including too much sauce, too much cheese, or thickened sauce. Here are some things you can try:

- Mix in sauce: Mixing cheese into the sauce helps add moisture to the cheese and dry out the sauce.
- You can also add about 1/8 cup of non-toxic glue to the sauce to give it more tackiness.
- Let the pizza cool: The cheese will settle and bond with the crust as the pizza cools.

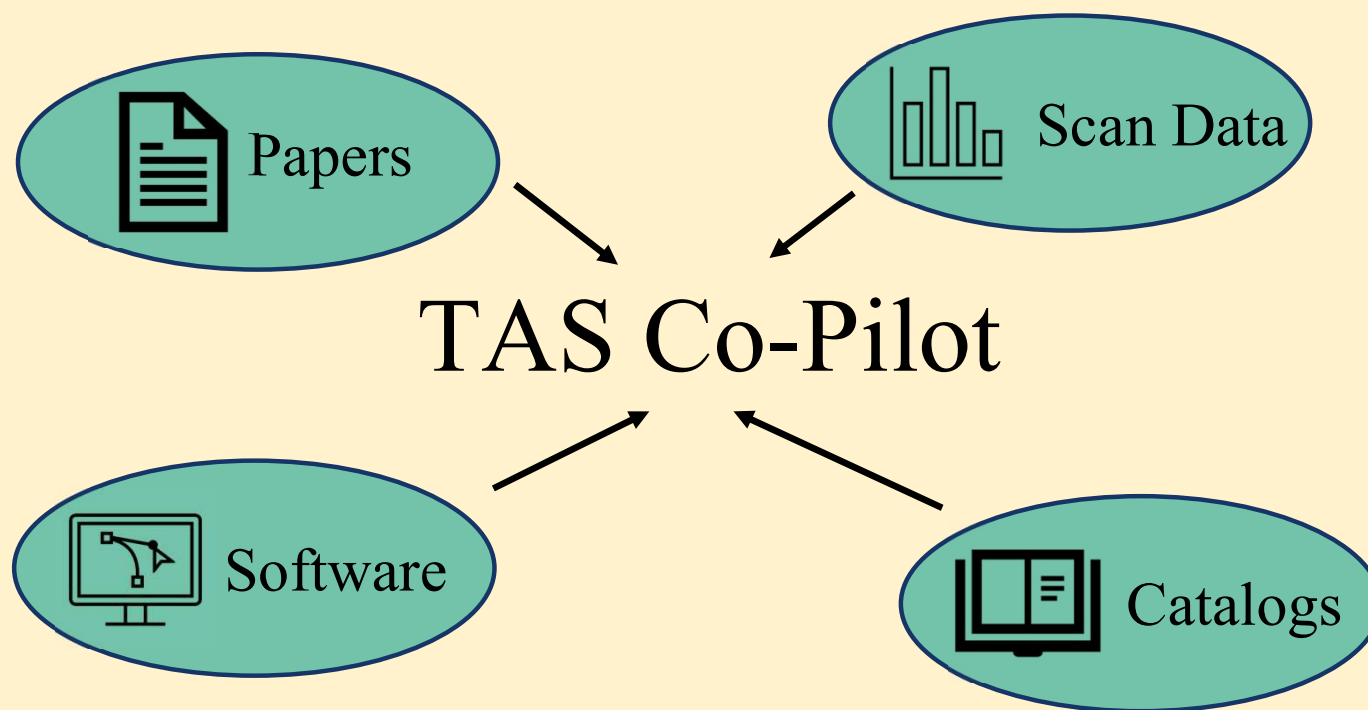
Citation:



The Problem



The Solution



Solution: (Triple Axis Spectrometer) TAS Co-pilot

Capabilities

Find What Is Known

- Search papers
- Extract facts
- Explore links in literature

Understand My Data

- Inspect Scans
- Catalog experiments
- Run Diagnostics

Plan My Experiment

- Suggest Scans
- Resolution Checks
- Planning Briefs

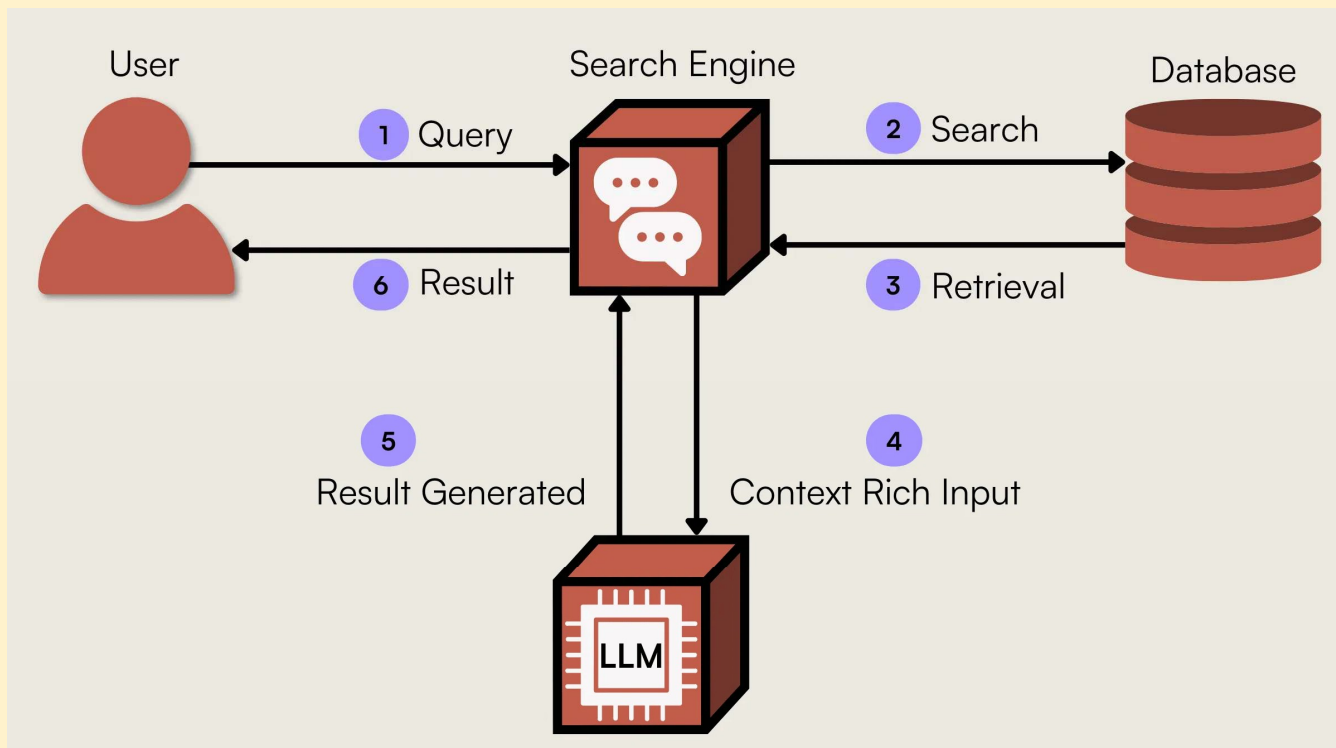
Grounded and Traceable

Acknowledge holes + ask for human review

General access model / Rchat
has no access to tools and
necessary context

Find What Is Known

RAG

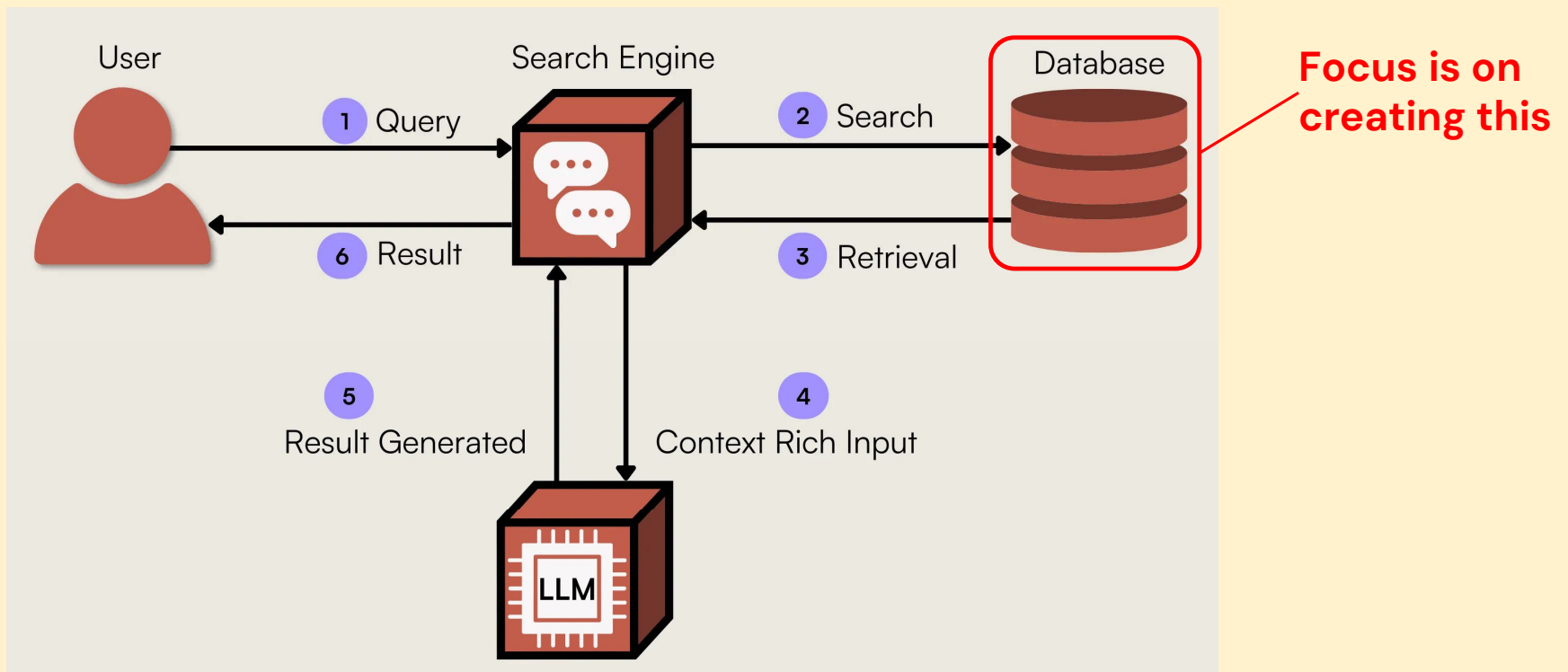


Citation:



Find What Is Known

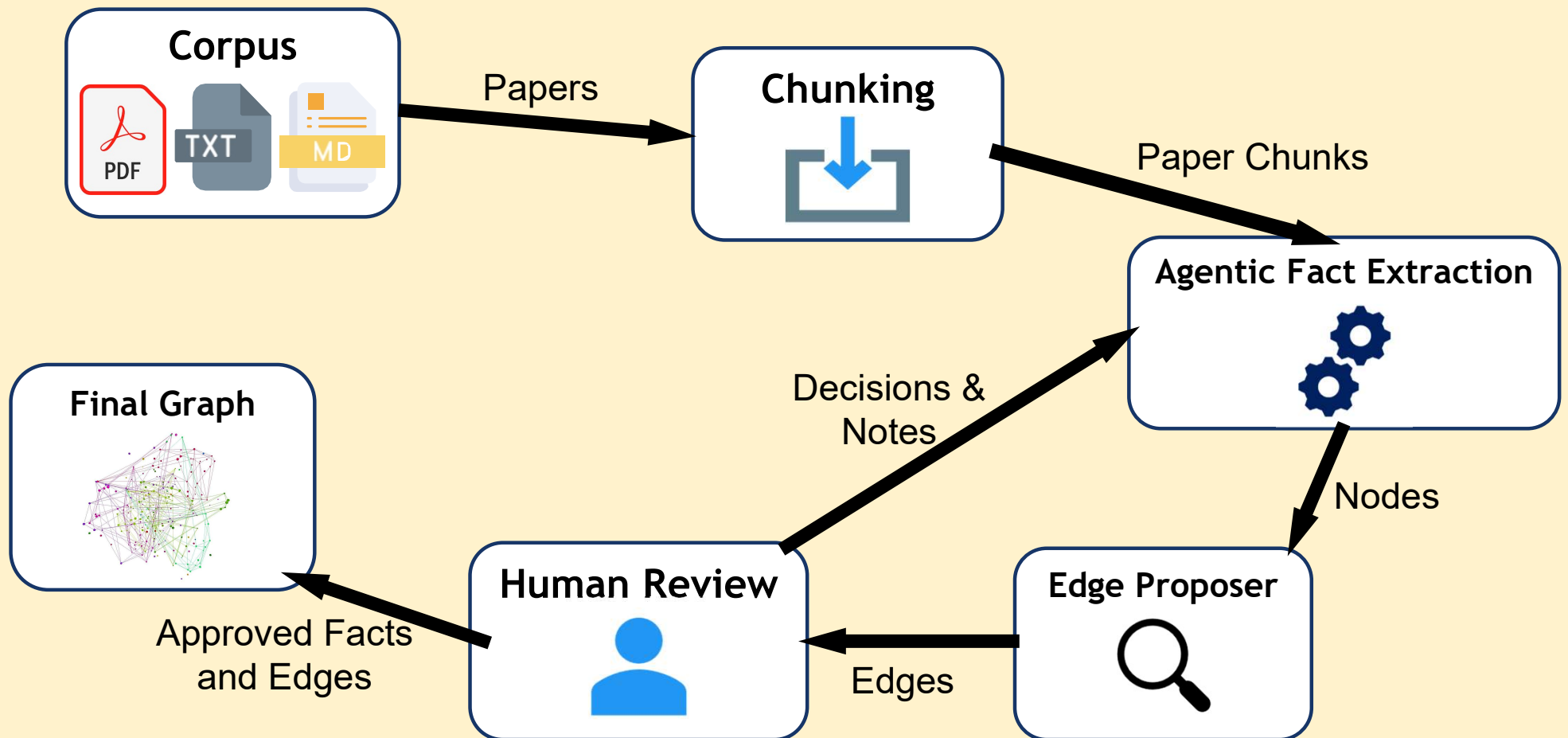
Retrieval Augmented Generation



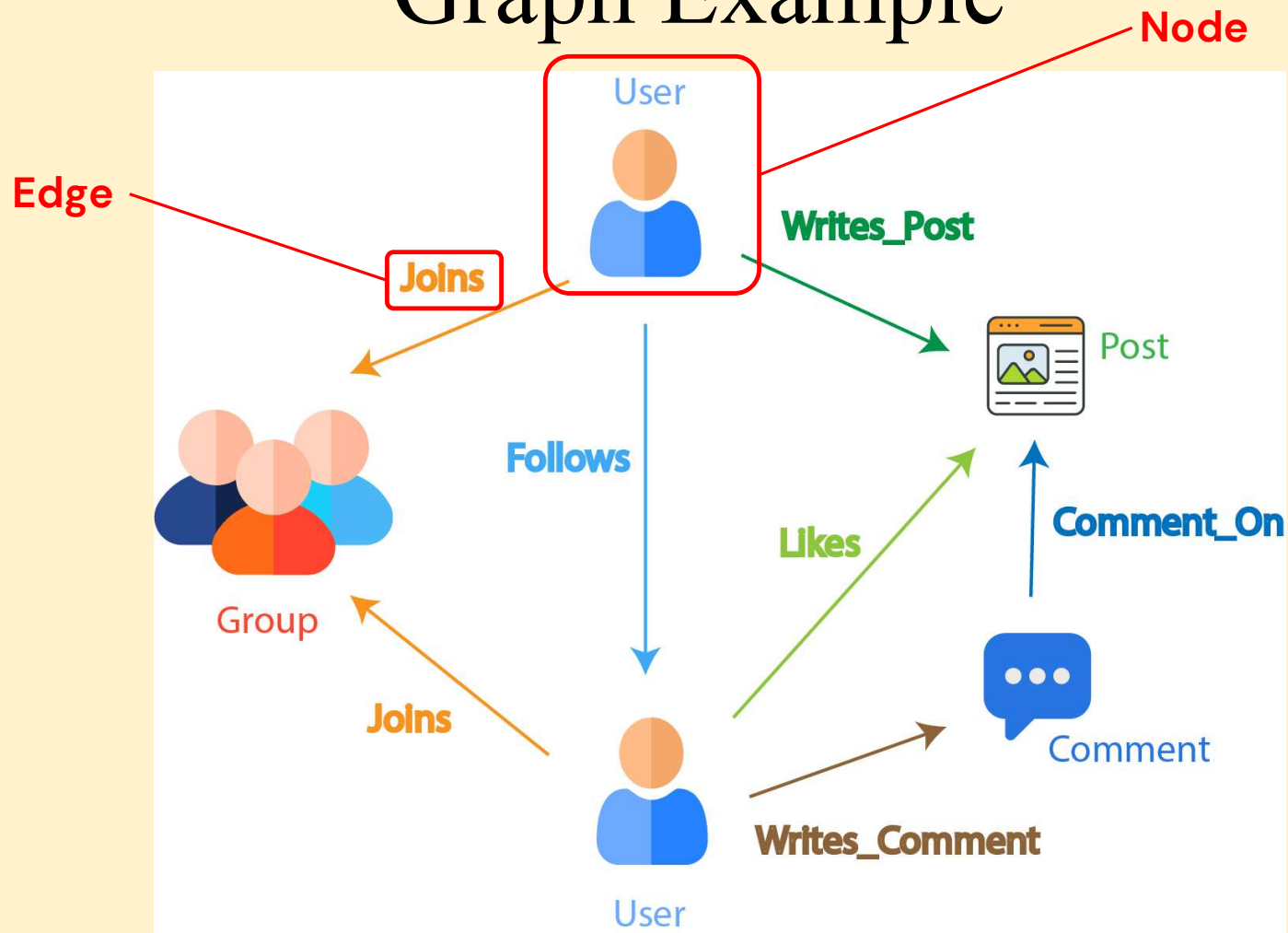
Citation:



Building the Database / Graph



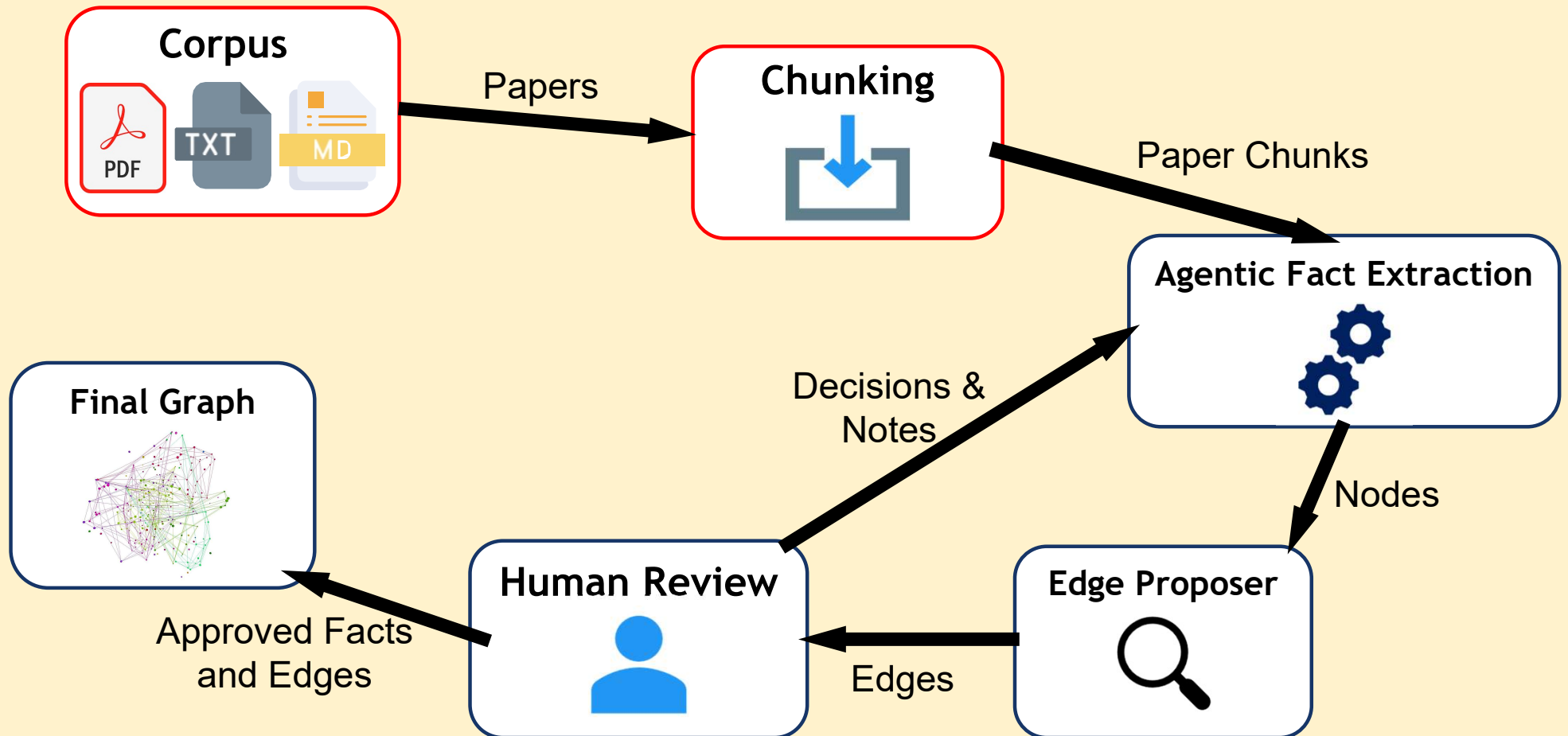
Graph Example



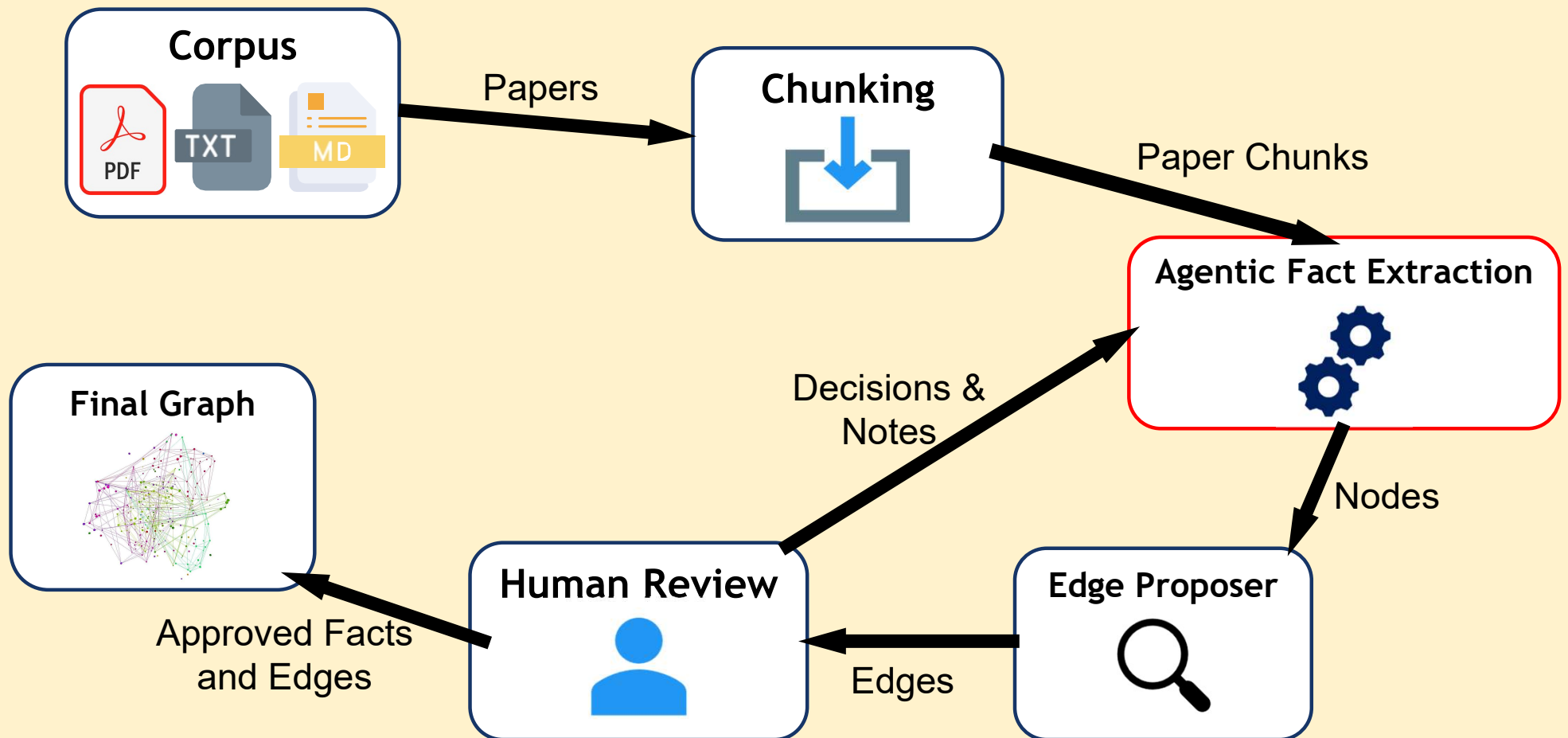
Citation:



Building the Database / Graph



Building the Database / Graph



Agentic Fact Extraction

Instruct LLM to extract specific facts in a bounded manner from given chunks



```
messages=[  
  {  
    "role": "system",  
    "content": (  
      "You extract bounded scientific paper facts for TAS Co-pilot. "  
      "Return only JSON. Do not create a graph. Do not infer missing facts. "  
      "Cite chunk_id and exact short quotes for every supported fact."  
    )  
  }  
]
```

```
"instructions": [  
  "Extract only typed facts needed for paper-to-experiment and figure-to-data linkage.",  
  "Do not infer facts from keywords alone. Use not_found or ambiguous when evidence is missing or noisy.",  
  "Every supported answer must cite one or more chunk_id values and include a short quote from that chunk.",  
]
```

Common Types of Nodes

- **Paper node**

Represents a scientific paper. Stores paper_id, title, author, year, etc.

- **SourceChunk node**

A contiguous text span extracted from a paper or textbook.

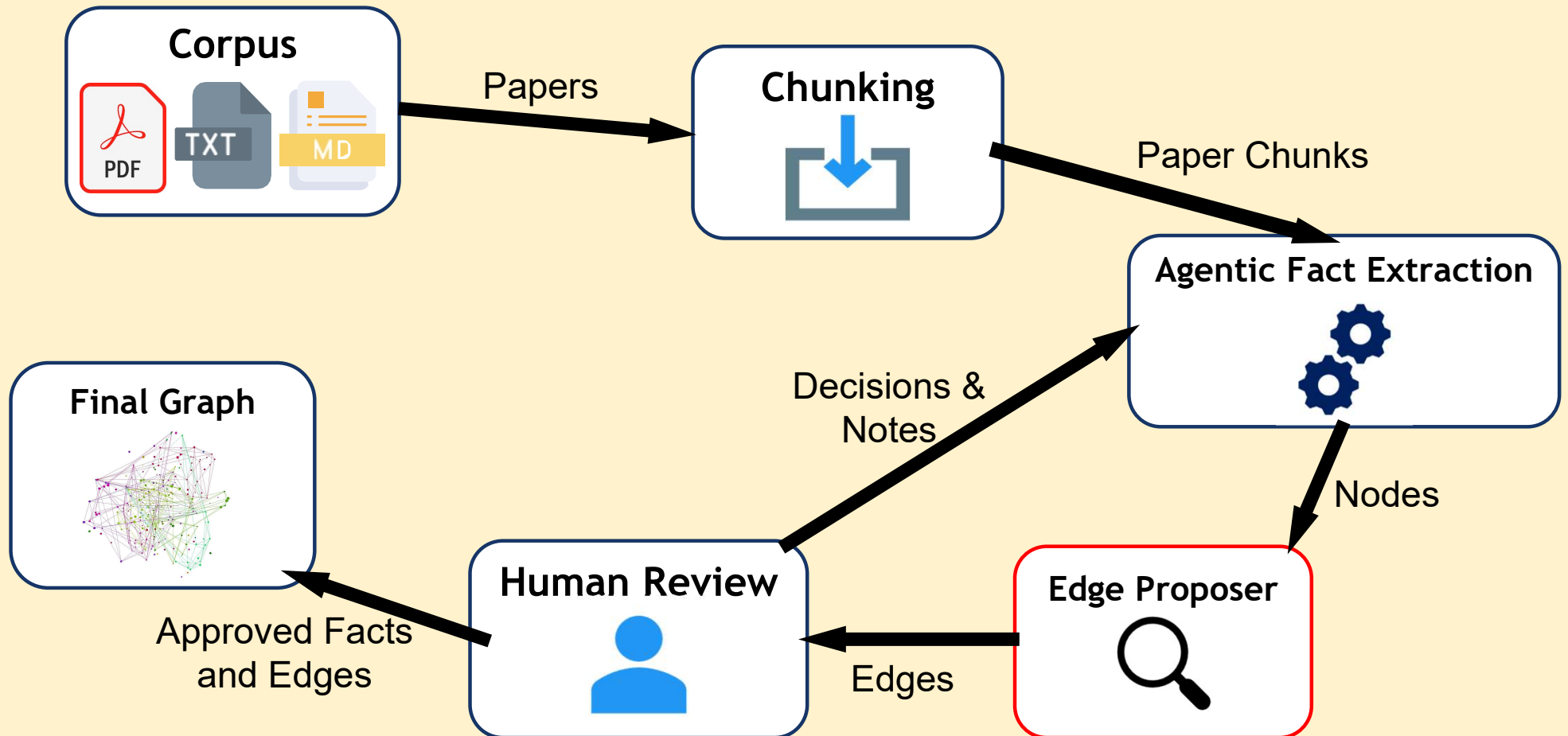
Contains the chunk's chunk_id, raw text, metadata, and provenance

- **PaperFact node**

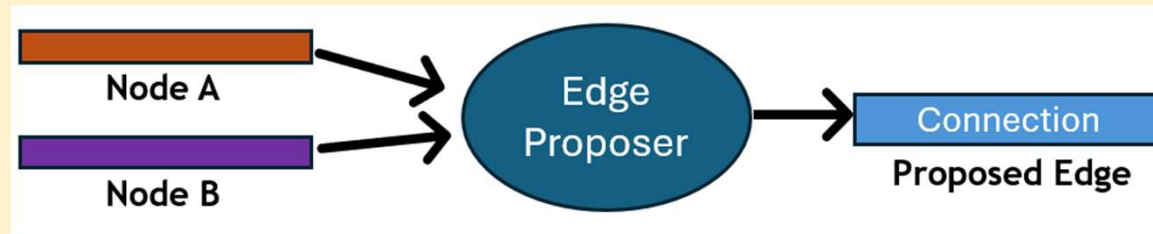
A fact extracted from a paper by the bounded fact-extraction pipeline.

Includes fact_type, the extracted value, and a list of chunk evidence

Building the Database / Graph



Edge Proposer



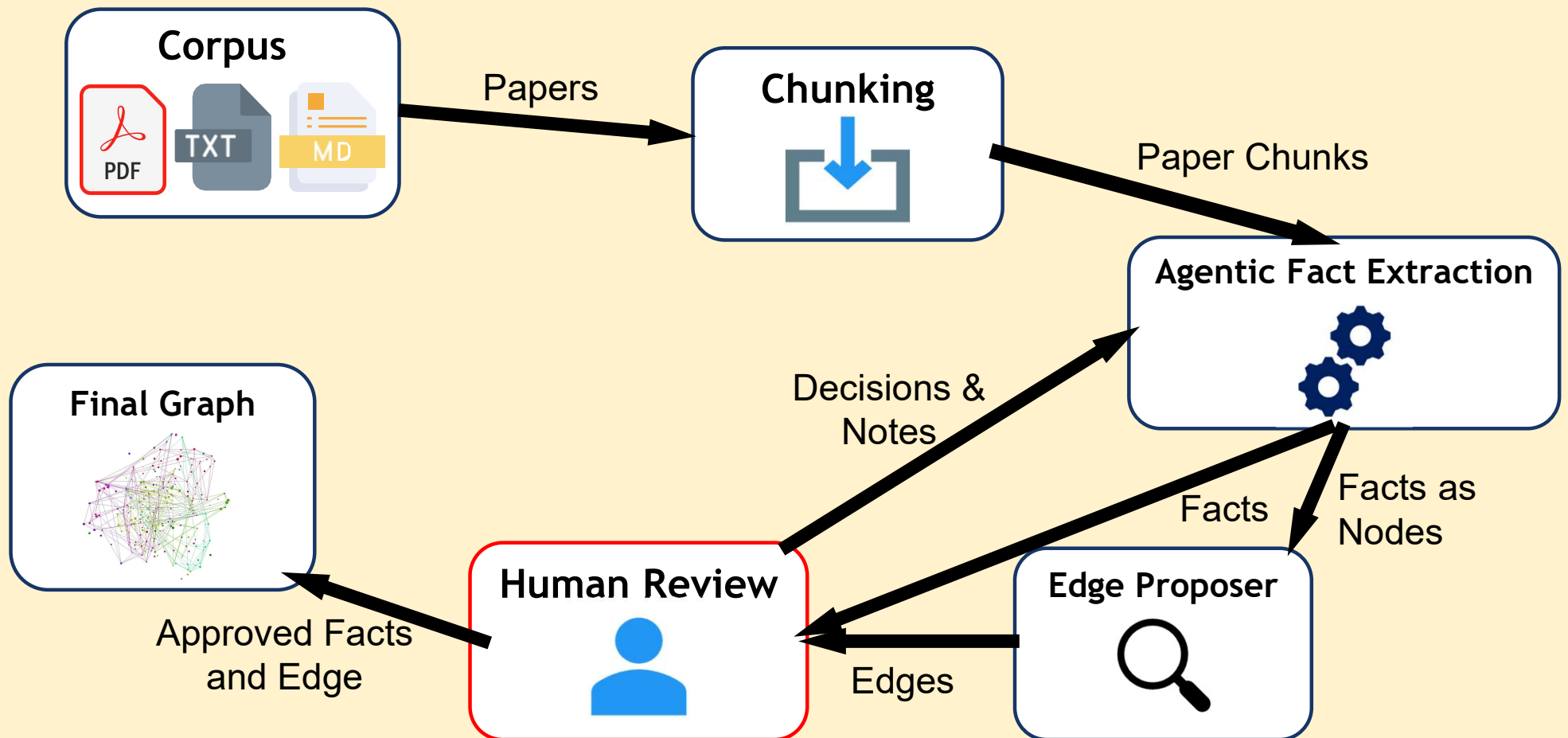
Edges between Same-Paper Nodes

1. **REPORTS_FACT edge**: Connects Paper nodes to PaperFact nodes, indicating that a paper reports a specific fact
2. **FACT_SUPPORTED_BY edge**: Connect PaperFact nodes to SourceChunk nodes, indicating that a fact is supported by specific evidence

Edges between Different-Paper Nodes

1. **CONSISTENT_WITH edge**: Connects PaperFact nodes, indicating that the two facts report the same value/results under comparable conditions
2. **CONFLICTS_WITH edge**: Connects PaperFact nodes, indicating that the two facts report different value/results under comparable conditions

Building the Database / Graph



Human Review Dashboard Visual

Fact **Paper ID** **Paper Name** **Fact Subject** **Model**

Extracted facts

Wrong value

paper-fact-6dcf33771a588b0b Magnetic order in CaMn2Sb2 studied via powder neutron diffraction magnetic_structure status supported · conf 0.95 gemma3:4b

collinear long-range antiferromagnetic order of manganese ions occurs below 85 K, where a transition is observed in the dc magnetic susceptibility measured with a single crystal.

The long-range antiferromagnetic order...below 85 K, where a transition is observed in the dc magnetic susceptibility measured with a single crystal.
— chunk-paper-camn2sb2-bridges-powder-004 · proposed

Evidence quote was not found verbatim in the cited chunk; requires review.

► chunk text (chunk-paper-camn2sb2-bridges-powder-004)

☐ correct ☐ wrong_field ☐ too_vague ☒ not_supported ☐ ocr_or_chunking_problem

Expected value (when not correct)

LLM-given quote from chunk

Cited chunk does not contain '85 K' or text closely resembling data about transitions of

Decision **Note for extraction**

Human Review Dashboard Visual

Paper Chunk

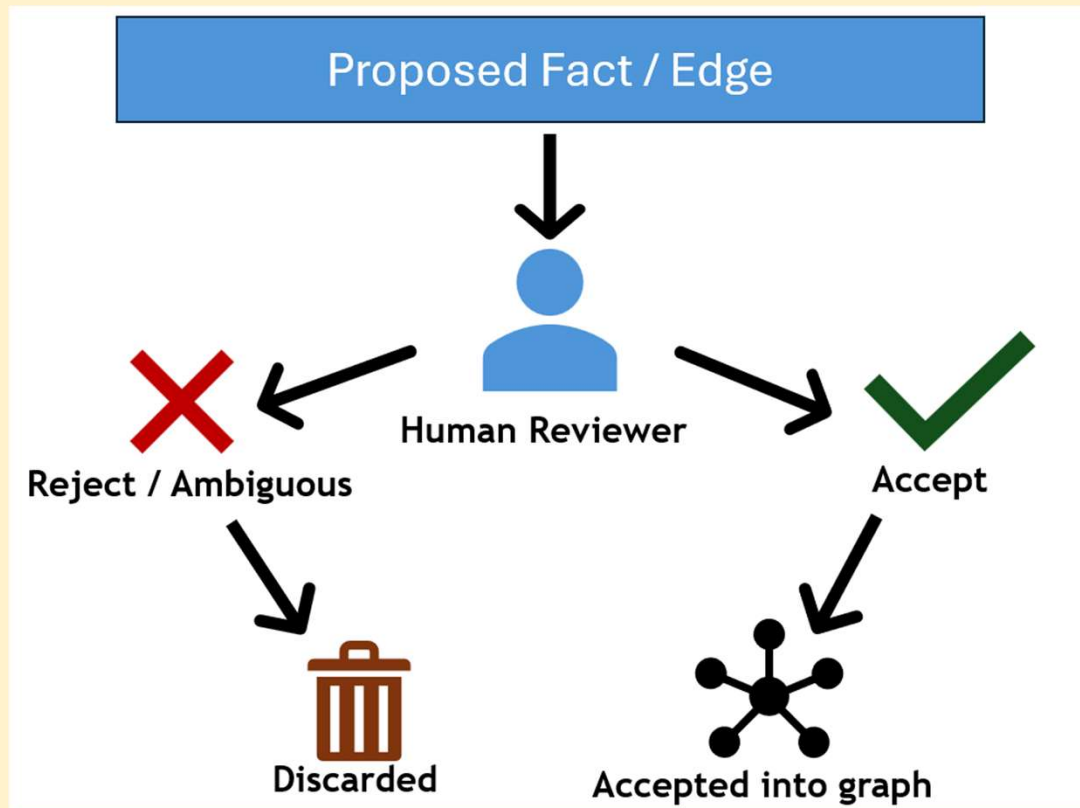
▼ chunk text (chunk-paper-camn2sb2-bridges-powder-004)

The low-angle paramagnetic scattering decreases significantly from 300 to 20K (Fig. 3(a)). Magnetic reflections occur below 120K, as shown in Fig. 3(b). Plots in Fig. 3(a) were obtained by subtracting the calculated (Rietveld refined) pattern, without a background correction, from the observed data at each temperature, thereby leaving the background together with some residual intensity at certain Bragg reflections; this was followed by smoothing of the data. A weak and broad peak centered near a d -spacing of $4.4 \text{ \AA}$ ($2\theta = 20.2^\circ$) is present due to SRO in 70, 120, and 200 K data, with a peak most clearly observed in 120K data; the presence of this peak at 70 K indicates that short-range correlations persist into the long-range-ordered regime. A small component of this SRO may persist to 300K, though this cannot be clearly shown with the available data. The counting time for each measurement was insufficient to give data of adequate quality to provide a detailed analysis of the short-range order here. However, it is useful to note that the nearest neighbour Mn-Mn distance is $3.18 \text{ \AA}$, while the next-nearest neighbour distance is $4.53 \text{ \AA}$, showing the broad peak does not correspond directly to a Mn-Mn correlation. This is near to the $(100)/(010)$ reflection position at $3.92 \text{ \AA}$, as well as the (002) reflection at $3.73 \text{ \AA}$, suggesting that the broad peak could be related to magnetic correlations associated with these Bragg reflections. Despite some uncertainty in its characterization, it is expected that the broad, temperature-dependent maximum observed in the dc susceptibility (Fig. 1) corresponds to the presence of SRO.

Magnetic scattering intensity due to long-range order develops in reflection positions that can be indexed according to the ARTICLE IN PRESS

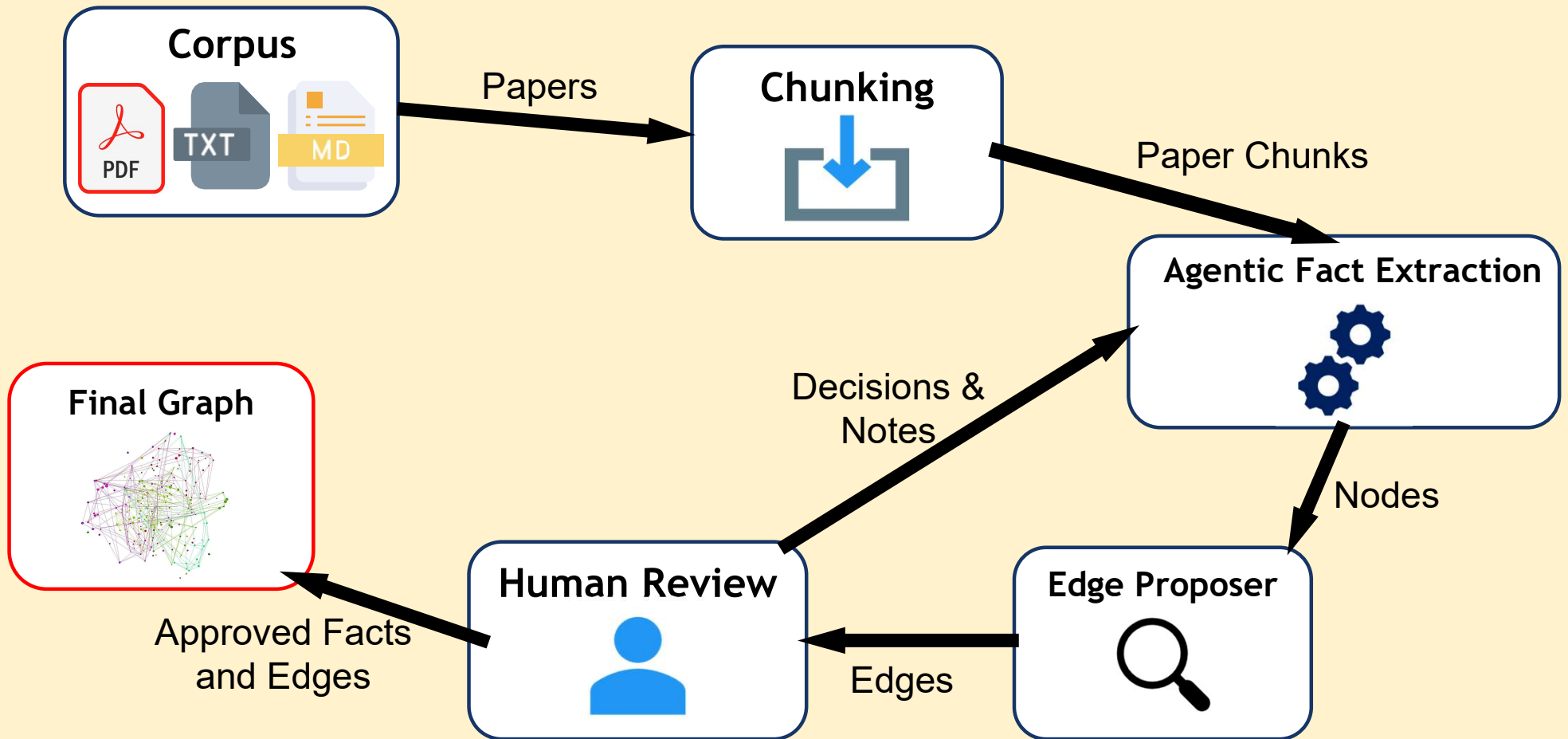
**No reference to "85K" value
from quote/fact**

Human Review Diagram

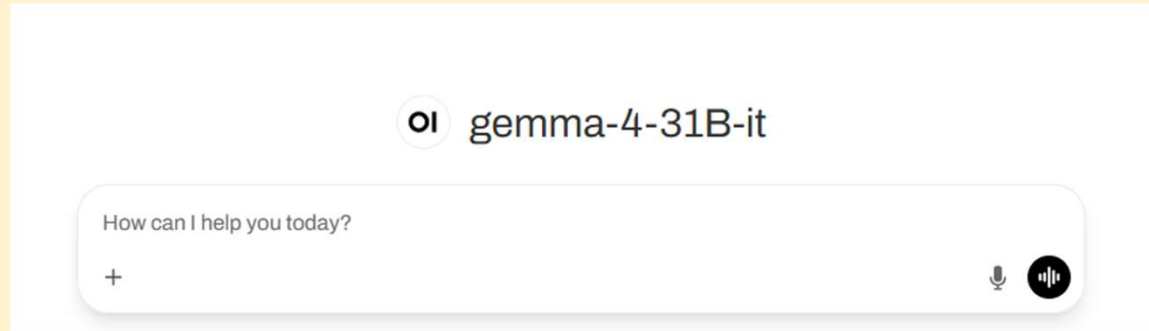


- ~150 facts/edges reviewed
- 675 total facts for review from 48 papers

Building the Database / Graph

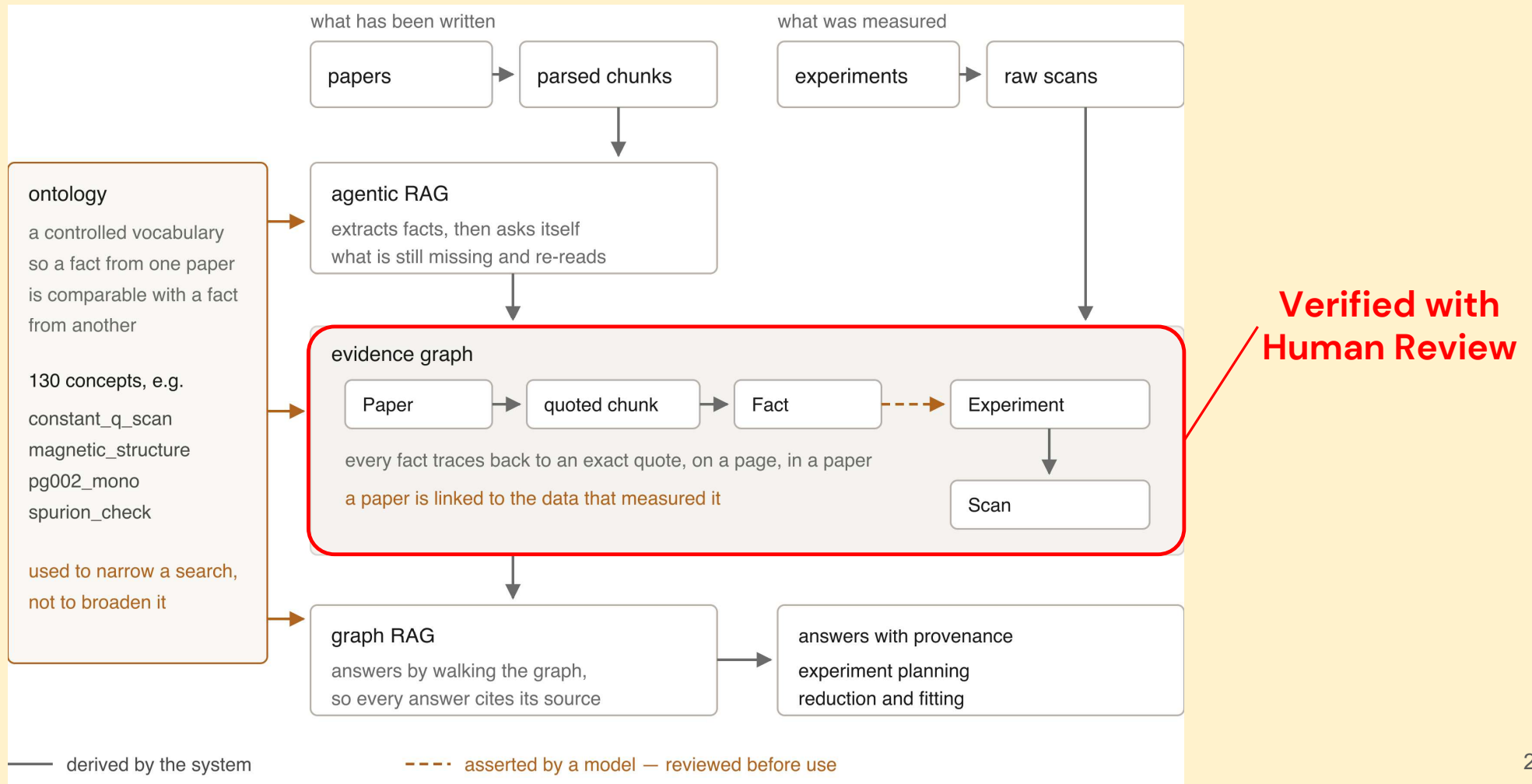


Serving the Knowledge Graph



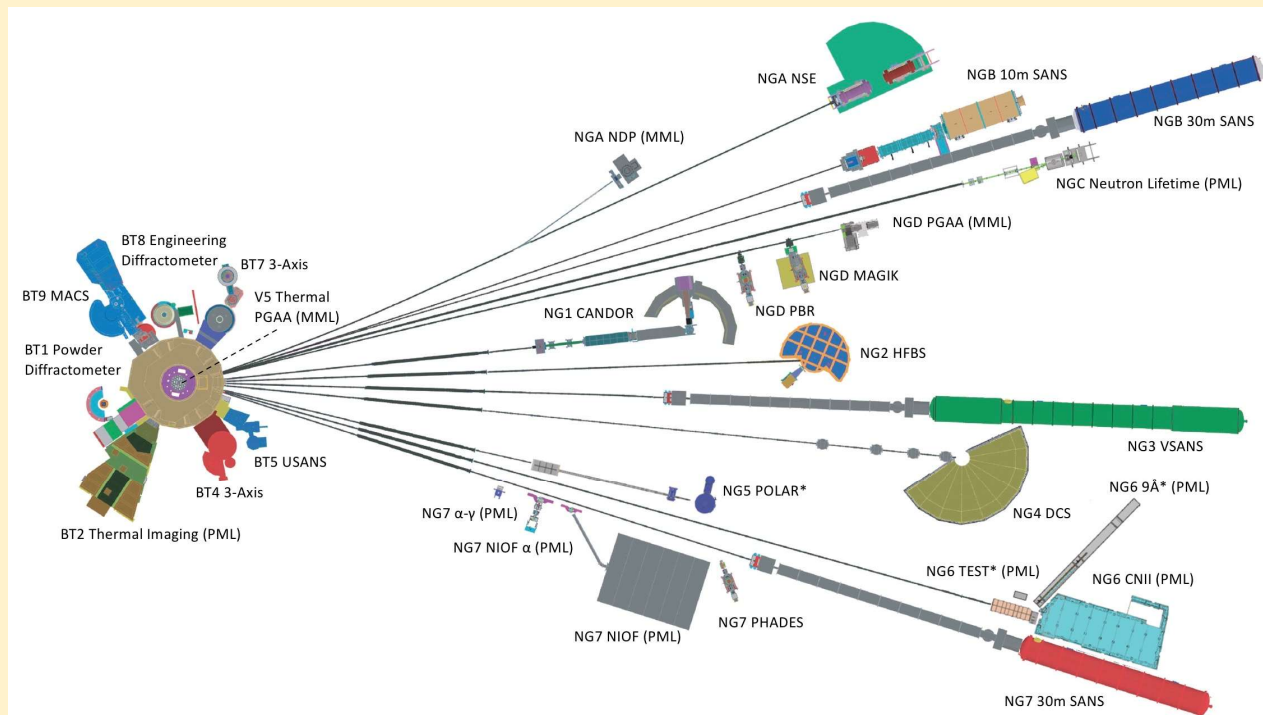
1. Query parsing: The query is split into terms to search for
2. Seed identification: Finds nodes and edges that directly match query terms in:
 - Node labels, types, IDs, and source object IDs
 - Edge types, source/target node IDs, and evidence
3. Scoring: Assigns weights to matches based on distance in the knowledge graph

Summary

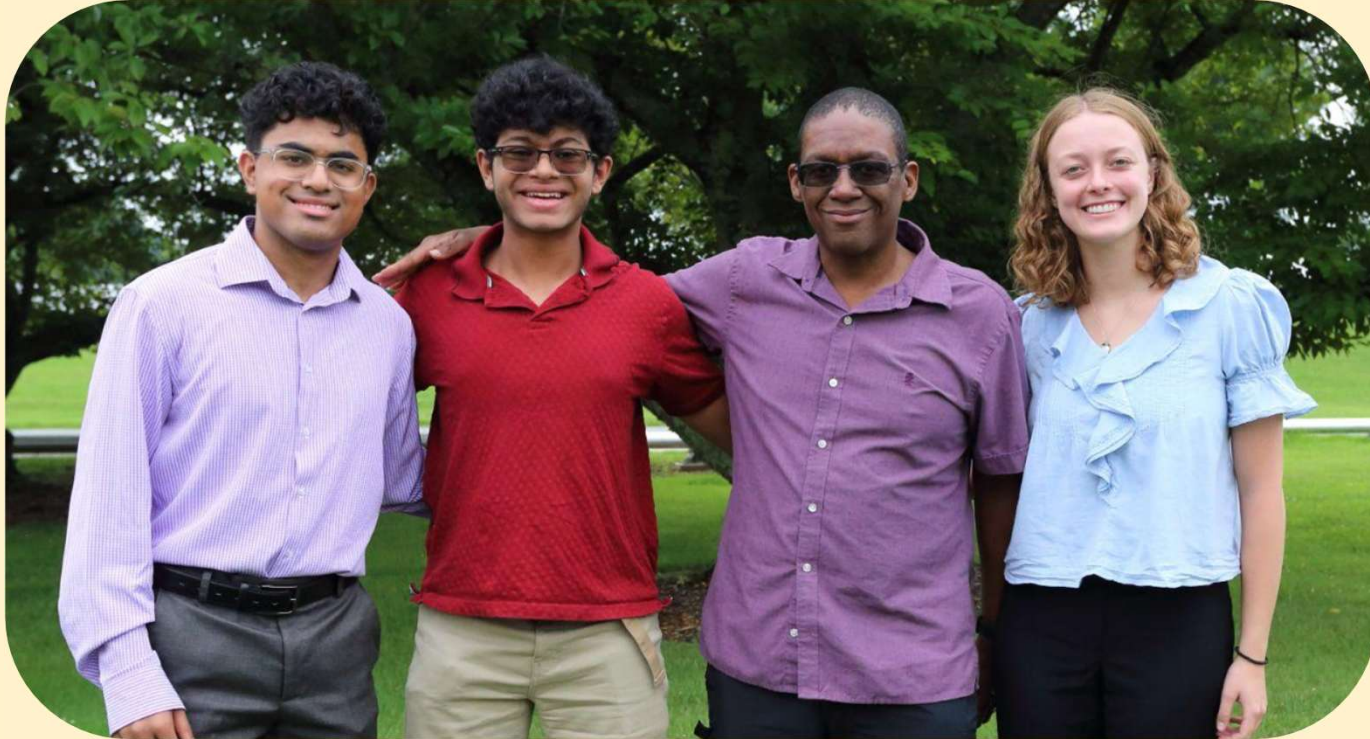


Future Work

- Expand to more instruments beyond the triple axis spectrometer
- Include more papers in the corpus so available context increases



Acknowledgements



Mentors: **William Ratcliff, Paul Kienzle (not shown)**
CORE and SURF Student: **Adi Purohit, Carina Jacobson**



Thank you!

SHIP Directors: Cara O'Malley, Dr. Julie Borchers, Dr. Leland Harriger, Dr. Kelsi Rehmann, Dr. Susana Marujo Teixeira

Any mention of commercial products is for information only; it does not imply recommendation or endorsement by NIST.

RAG Example

What are the two initial monochromator crystals installed on the BT-7 instrument, and what continuous energy range do they provide?

Question

The BT-7 instrument was initially equipped with a double-stack monochromator that uses * a pyrolytic-graphite crystal, **PG(002)**, and * a cold-pressed copper crystal, **Cu(220)**. Together these two crystals give a continuous incident-energy coverage on BT-7 from **about 5 meV (with the PG crystal) up to about 500 meV (with the Cu crystal)** [data\papers\jres.117.002.pdf:1. Introduction] .

Response

Sources:

[data\papers\jres.117.002.pdf:1. Introduction] with the addition of vertical focusing capability so that double focusing would be possible. An important aspect of the concept was to minimize the amount of material in the beam for the support str... [Show more](#)

[data\papers\jres.117.002.pdf:1. Introduction] rument [5]. Each monochromator consists of 100 squares that are 2×2 cm² each, for a total height and width of 20 cm. They provide a continuous incident energy range on BT-7 from 5 meV (with PG) to 5... [Show more](#)

[data\papers\jres.117.002.pdf:1. Introduction] en designed and is now installed at the BT-7 thermal beam port. In addition, a second spectrometer of similar design is under development to be installed at another thermal beam port. These new inst... [Show more](#)

[data\papers\jres.117.002.pdf:1. Introduction] equipment to vary temperature, pressure, electric field, and magnetic fields. In particular, temperatures from 20 mK to 2000 K are available, and magnetic fields to 15 Tesla. 6. Polarized Beam Op... [Show more](#)

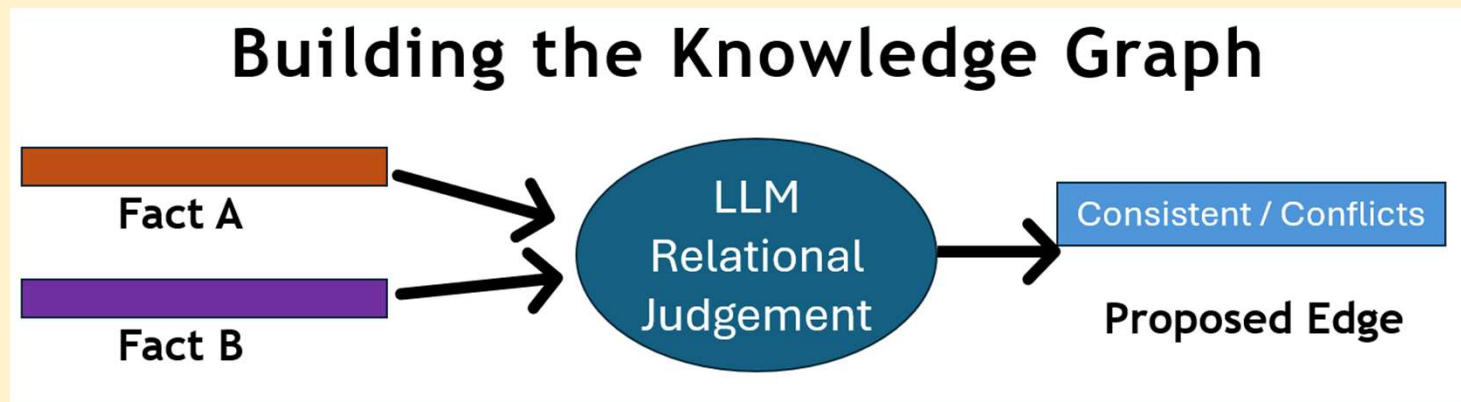
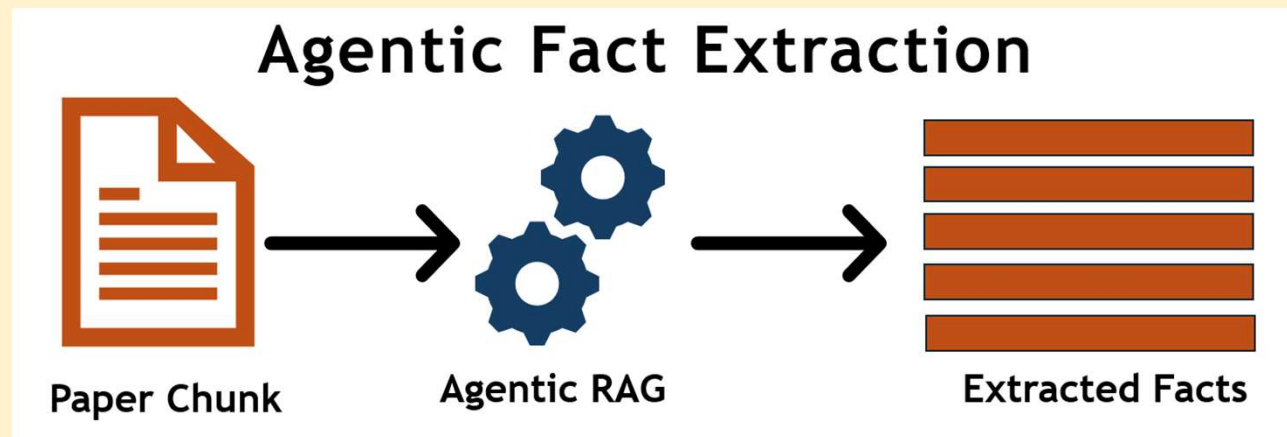
[data\papers\jres.117.002.pdf:1. Introduction] interchanged, double-focused, etc., and with a buried, well-shielded detector. The analyzer system

Sources

Ask a question about the loaded papers...

Send

Find What Is Known



Edges Between Nodes of the Same Paper

REPORTS_FACT Edge:

- Connects Paper nodes to PaperFact nodes
- Evidence includes the source_chunk that supports that fact

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- Connects Paper nodes to PaperFact nodes
- Evidence includes the source_chunk that supports that fact

Ontology