

# Retrieval-augmented Generation on Graph-structured Data



Yu Wang<sup>1</sup>



Haoyu Han<sup>2</sup>



Harry Shomer<sup>2</sup>



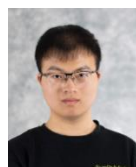
Kai Guo<sup>2</sup>



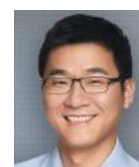
Yongjia Lei<sup>1</sup>



Jiayuan Ding<sup>4</sup>



Xianfeng Tang<sup>3</sup>



Qi He<sup>3</sup>



Jiliang Tang<sup>2</sup>

University of Oregon<sup>1</sup>  
Michigan State University<sup>2</sup>  
Amazon<sup>3</sup>  
Hippocratic AI<sup>4</sup>



SDM25-GraphRAG

# Addressing real-world tasks desire knowledge

Just can't remember.....



What are they talking about?



What should I look next?

Home & Kitchen > Kitchen & Dining > Coffee, Tea & Espresso > Espresso Machine & Coffeemaker Combos

**L'OR Barista System Coffee and Espresso Machine Combo by Philips, Matte Black**

Visit the L'OR Store  
4.2 ★★★★★ (2,376)  
500+ bought in past month

**\$189.00**  
Or **\$32.58/mo** (6 mo). Select from 2 plans  
prime  
FREE Returns

A gift for you: Unlock a \$100 Amazon Gift Card on approval for Prime Visa. Plus get 5% back on your Amazon purchases.

Style: **Matte Black**

Matte Black	Matte Black/Pre...	Matte Grey	Matte Grey Machine *...
\$189.00 FREE Delivery Sunday	\$159.00 FREE Delivery Sunday	\$219.00 FREE Delivery Sunday	\$199.00 FREE Delivery Sunday

Click to see full view

Brand: L'OR  
Color: Black  
Product Dimensions: 16"D x 7"W x 11"H  
Special Feature: Manual  
Coffee Maker Type: Espresso Machine

**Add a Protection Plan:**  
☐ 3-Year Protection Plan for \$28.99  
☐ 4-Year Protection Plan for \$38.99  
☐ Complete Protect: One plan covers all eligible past and future purchases (Renews Monthly Until Cancelled) for \$16.99/month

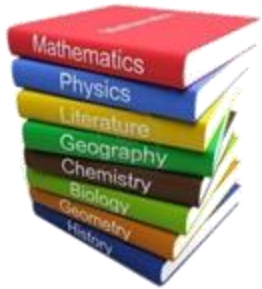


Query/Task Request

**Missing Knowledge!**

# Real-world knowledge is so much!

## Textbook Knowledge Base



**158 million books**

[ISBN DB 2023](#)

## Internet Knowledge Base



**1.1 billion websites**

[Musemind 2024](#)

## Neural Knowledge Base



**405 billion parameters**

[Hugging Face 2024](#)



 **2.5 petabytes, 1 billion books**

- We remember meanings, not details.
- We forget on purpose.
- Tiny active memory, Larger long-term memory.

**Retrieval Knowledge to Augment  
Downstream Task is Rather Important!**

# Retrieving External Knowledge

## Open-book Exam

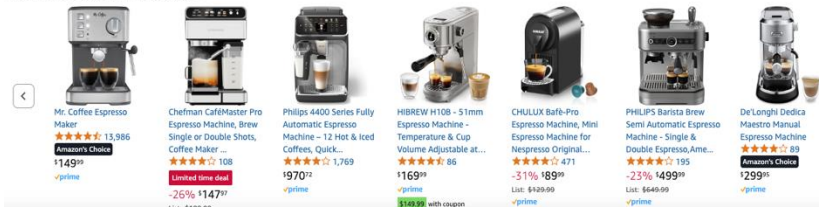


## Online Shopping

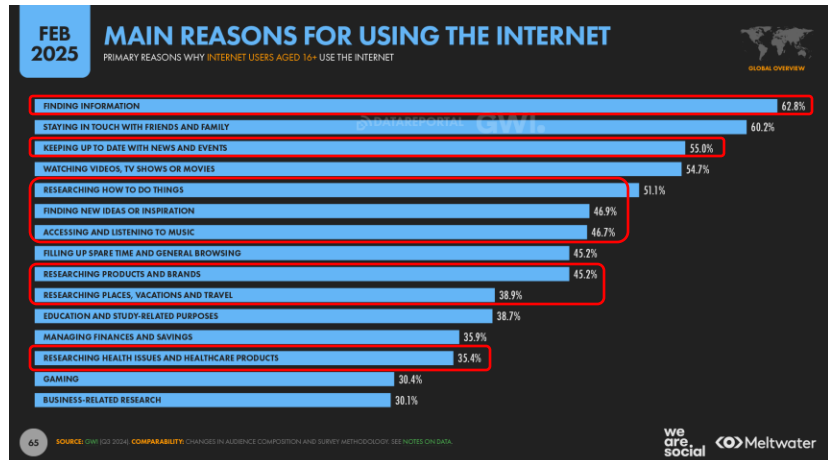
L'OR products customers bought together



Based on your recent views

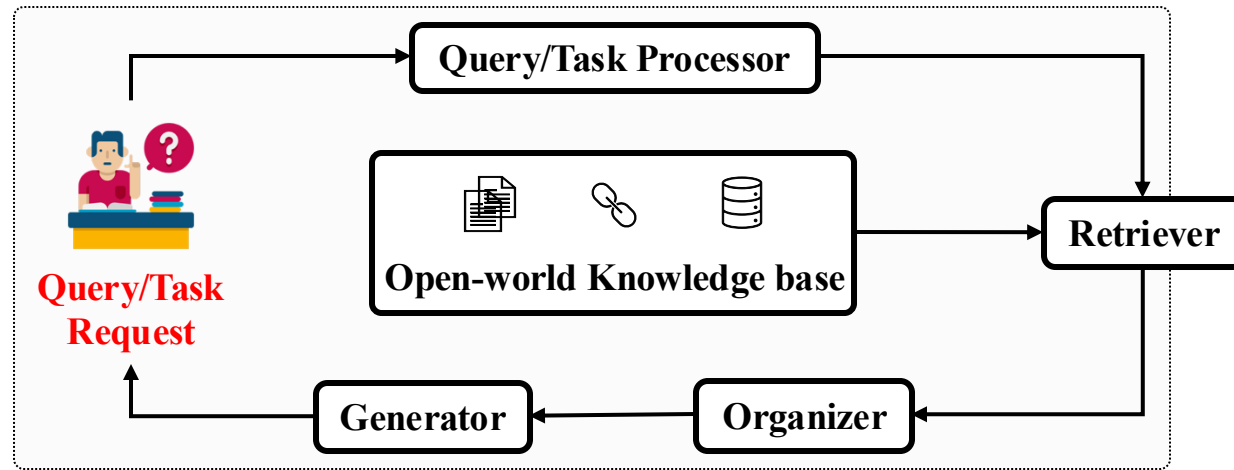


## Google Search

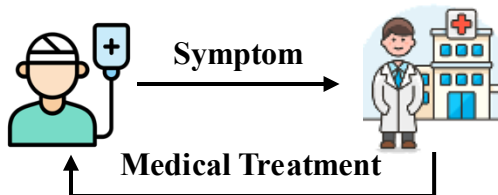




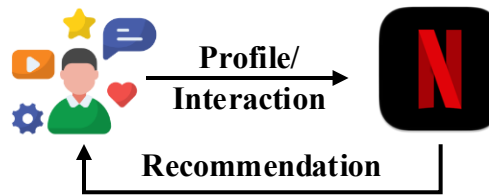
# Retrieval-augmented Generation (RAG)



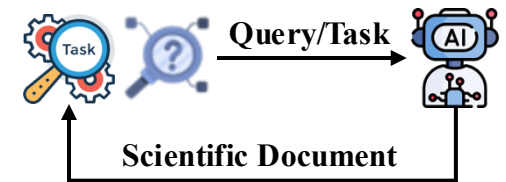
Query  $Q$



Any idea why I might be sick?



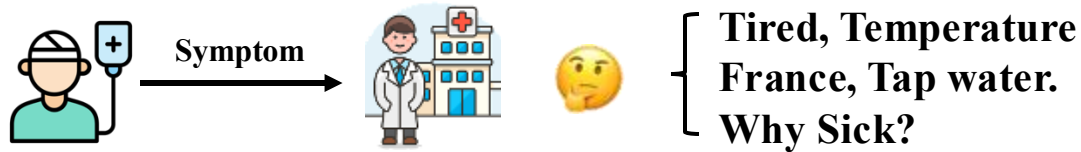
Can you recommend a mouse repellent that has a nice smell?



Find me papers that discuss improving condensers performance

# Retrieval-augmented Generation (RAG)

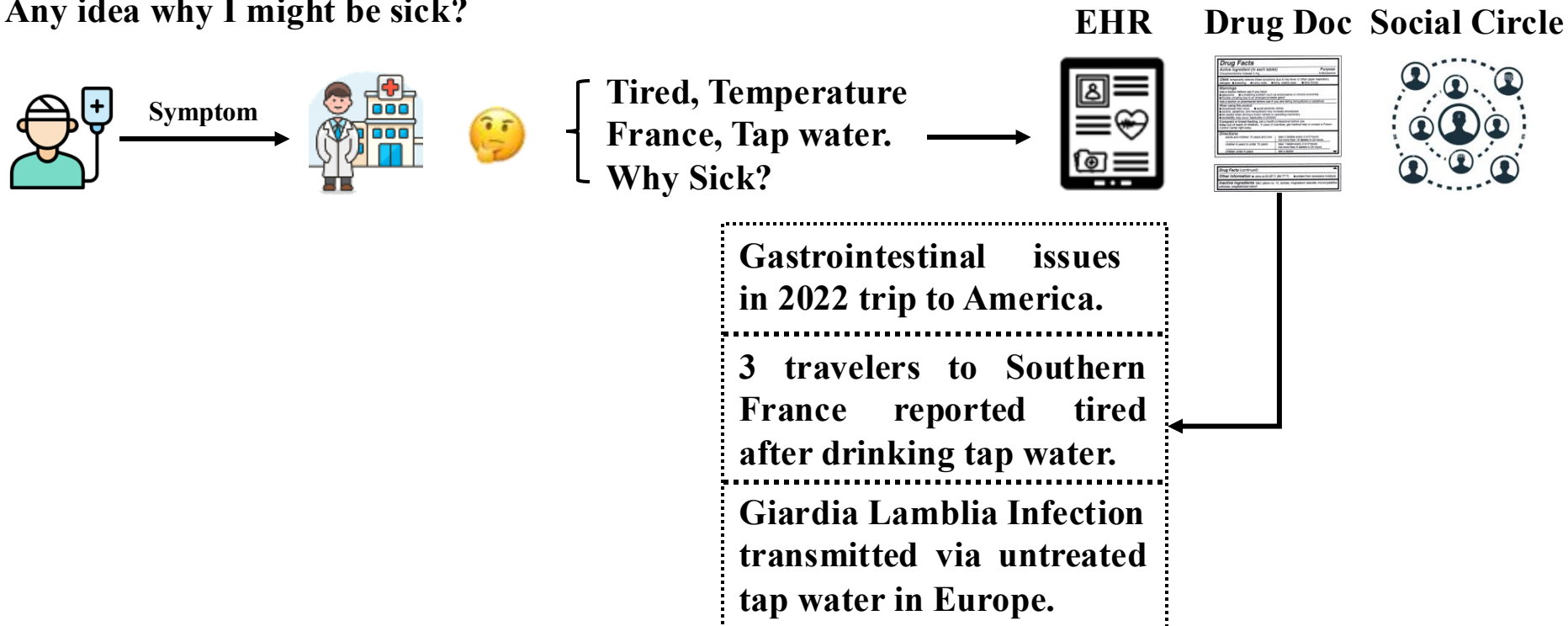
Really tired.  
Temperature is over 100.  
Recently in France.  
Drank a lot of tap water there.  
Any idea why I might be sick?



$$\hat{Q} = \Omega^{\text{Processor}}(Q)$$

# Retrieval-augmented Generation (RAG)

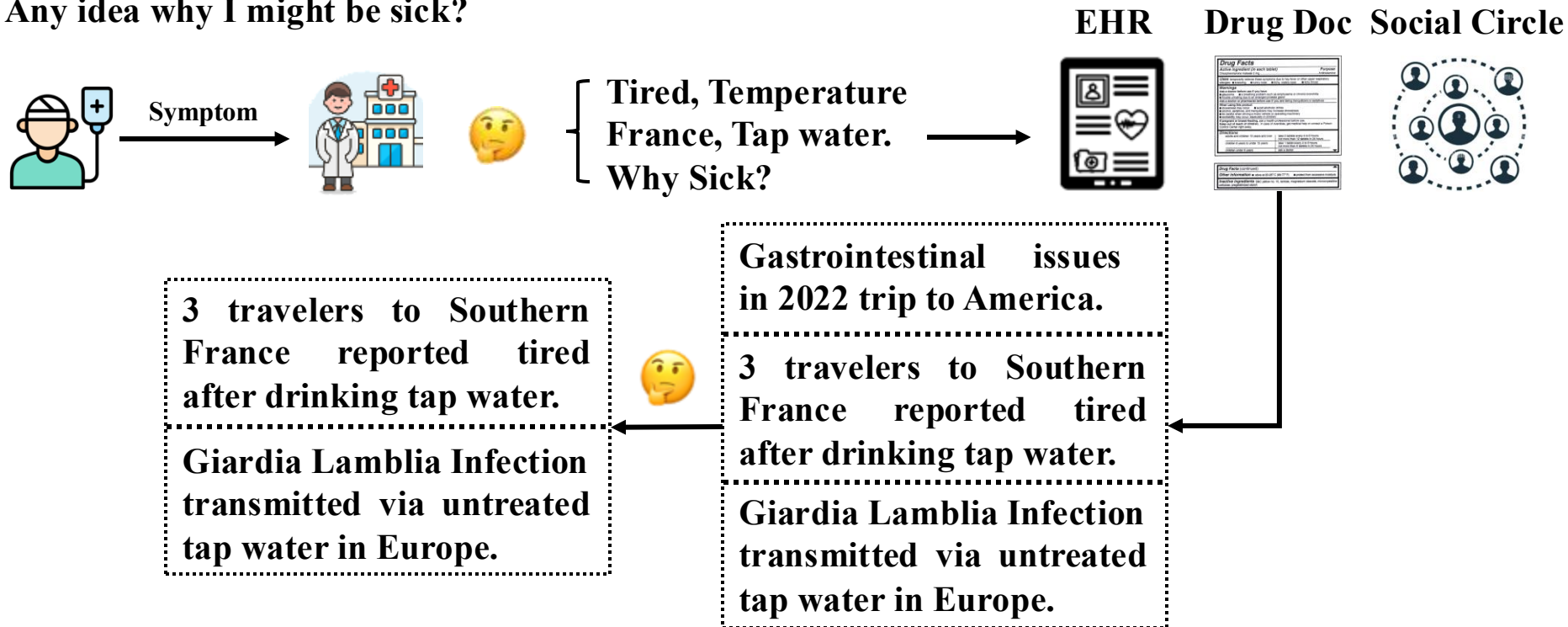
Really tired.  
Temperature is over 100.  
Recently in France.  
Drank a lot of tap water there.  
Any idea why I might be sick?



$$\hat{C} = \Omega^{\text{Retriever}}(\hat{Q}, C)$$

# Retrieval-augmented Generation (RAG)

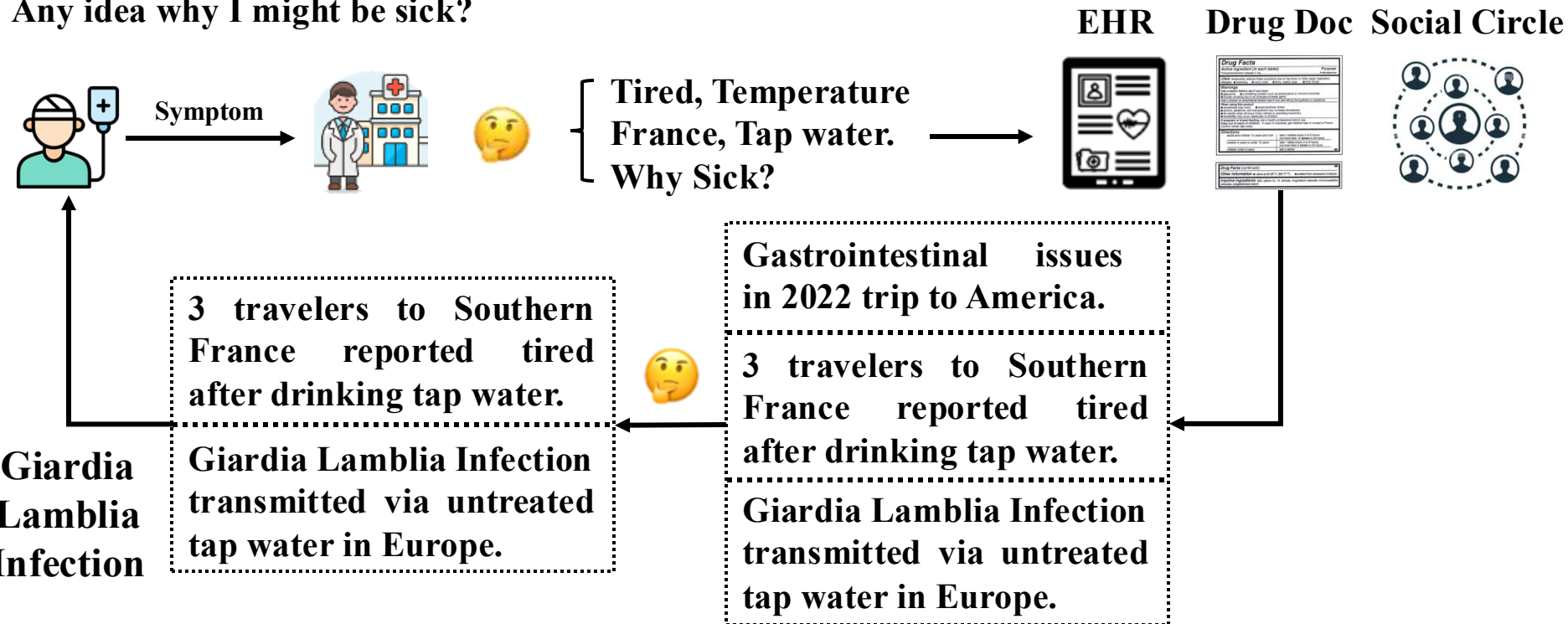
Really tired.  
Temperature is over 100.  
Recently in France.  
Drank a lot of tap water there.  
Any idea why I might be sick?



$$\hat{C} = \Omega^{\text{Organizer}}(\hat{Q}, C)$$

# Retrieval-augmented Generation (RAG)

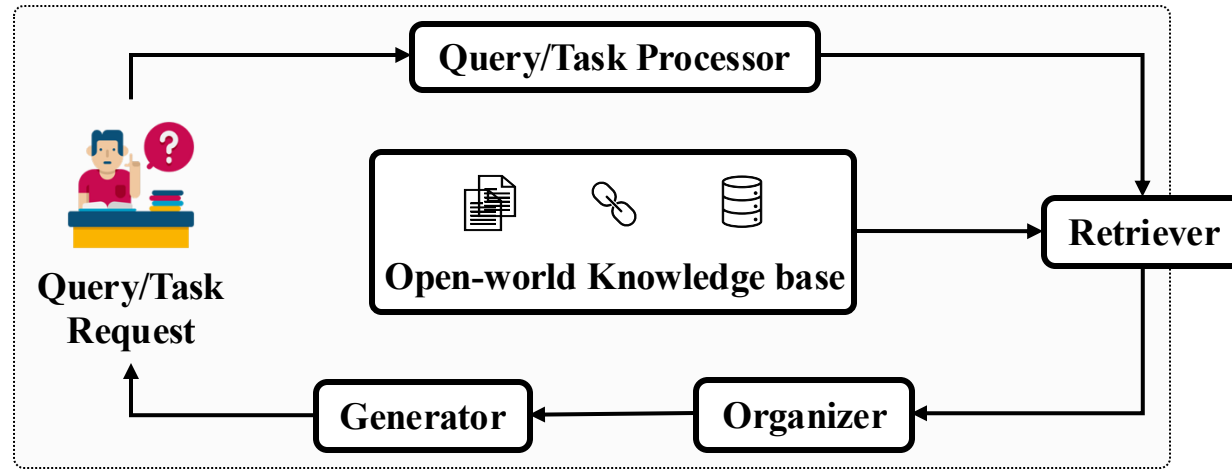
Really tired.  
Temperature is over 100.  
Recently in France.  
Drank a lot of tap water there.  
Any idea why I might be sick?



$$A = \Omega^{\text{Generator}}(\hat{Q}, \hat{C})$$



# Retrieval-augmented Generation (RAG)



(1) Query  $Q$

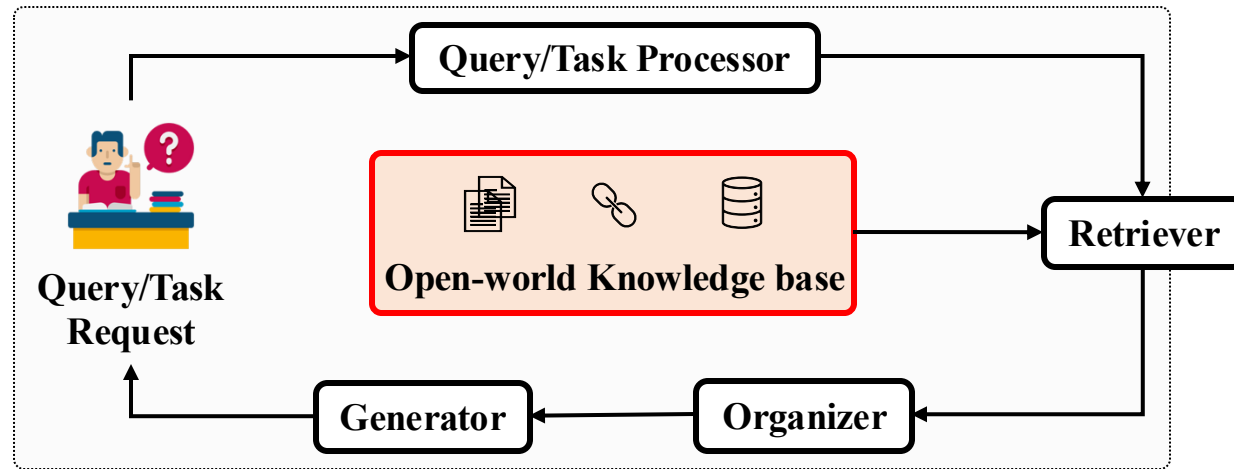
(2)  $\hat{Q} = \Omega^{\text{Processor}}(Q)$

(4)  $C = \Omega^{\text{Retriever}}(\hat{Q}, G)$

(5)  $\hat{C} = \Omega^{\text{Organizer}}(\hat{Q}, C)$

(6)  $A = \Omega^{\text{Generator}}(\hat{Q}, \hat{C})$

# Retrieval-augmented Generation (RAG)



(1) Query  $Q$

(2)  $\hat{Q} = \Omega^{\text{Processor}}(Q)$

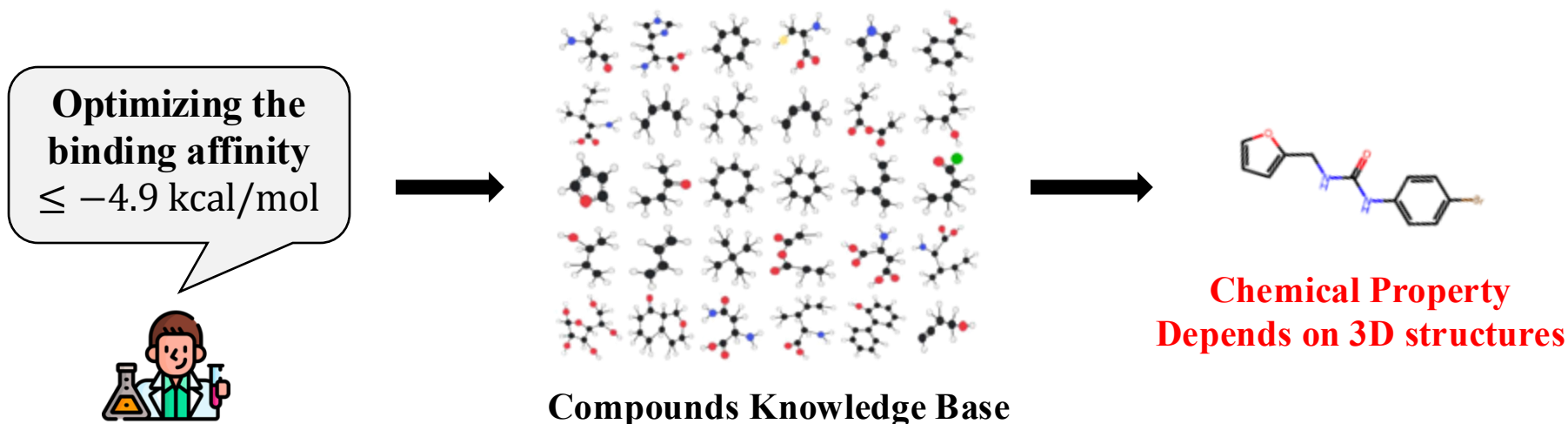
(4)  $C = \Omega^{\text{Retriever}}(\hat{Q}, G)$

(5)  $\hat{C} = \Omega^{\text{Organizer}}(\hat{Q}, C)$

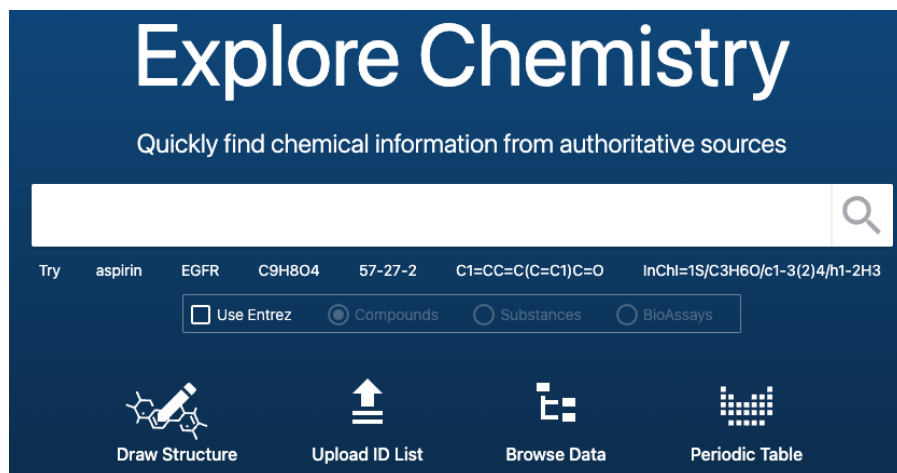
(6)  $A = \Omega^{\text{Generator}}(\hat{Q}, \hat{C})$

**Real-world knowledge can be extremely complex and heterogeneous!**

# Retrieval-augmented Generation (RAG) – Drug Design

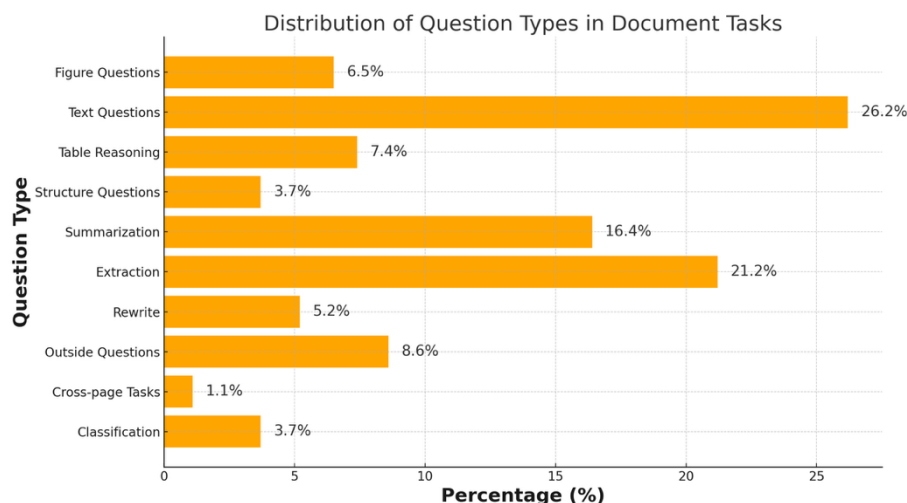
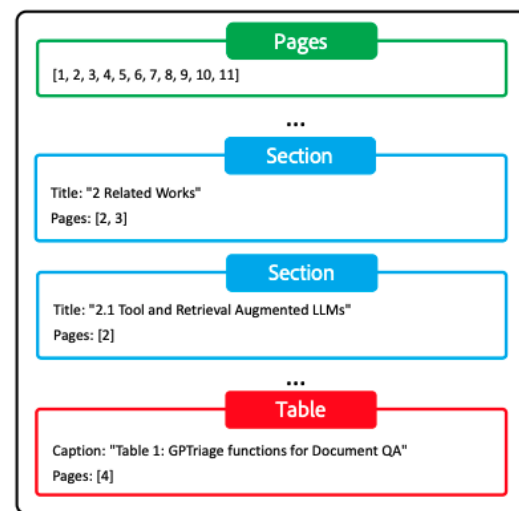
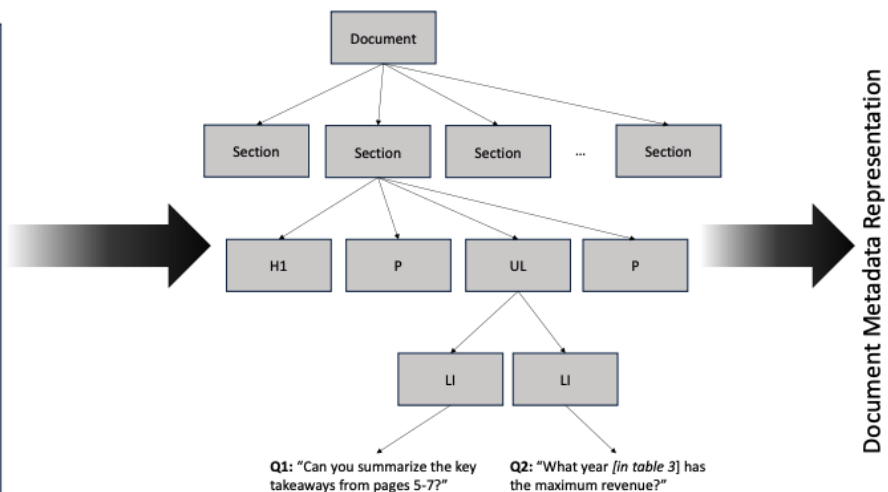


PubChem



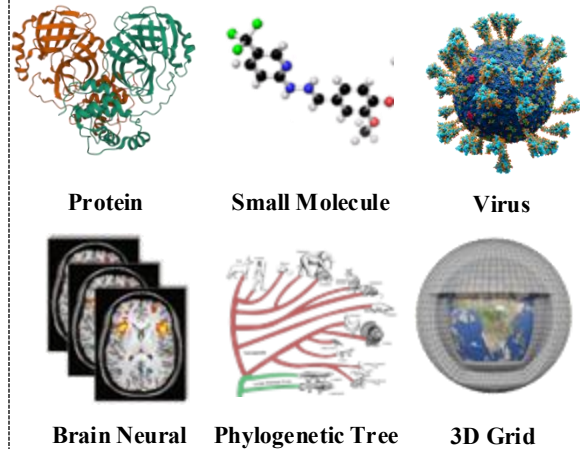
- **119M** Compounds
- **329M** Substances
- **297M** Bioactivities
- **42M** Literature
- **54M** Patents [pubchem](https://pubchem.ncbi.nlm.nih.gov/)

# Retrieval-augmented Generation (RAG) – Document

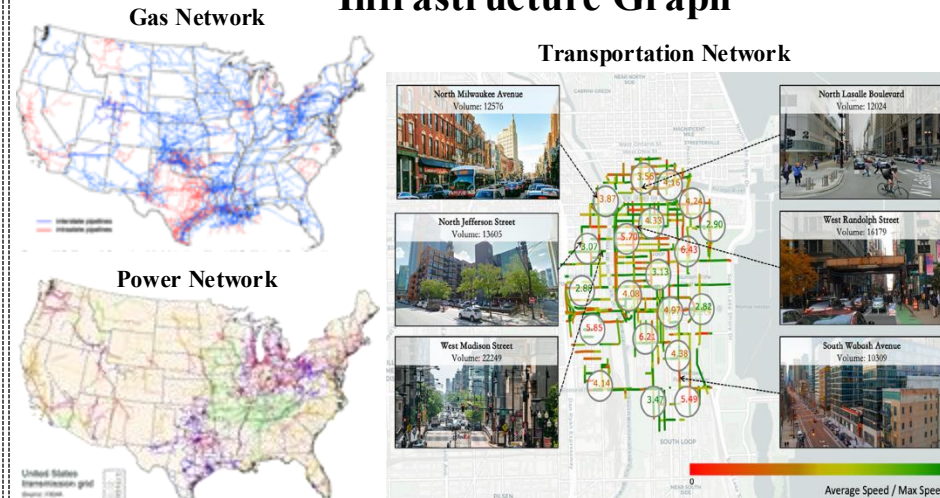


# Heterogeneous knowledge can be represented as Graph

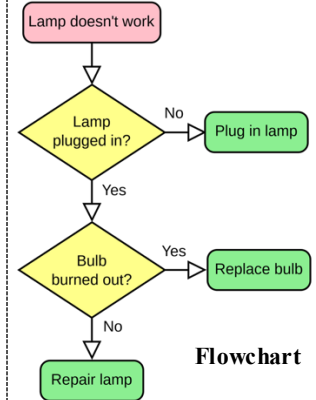
## Scientific Graph



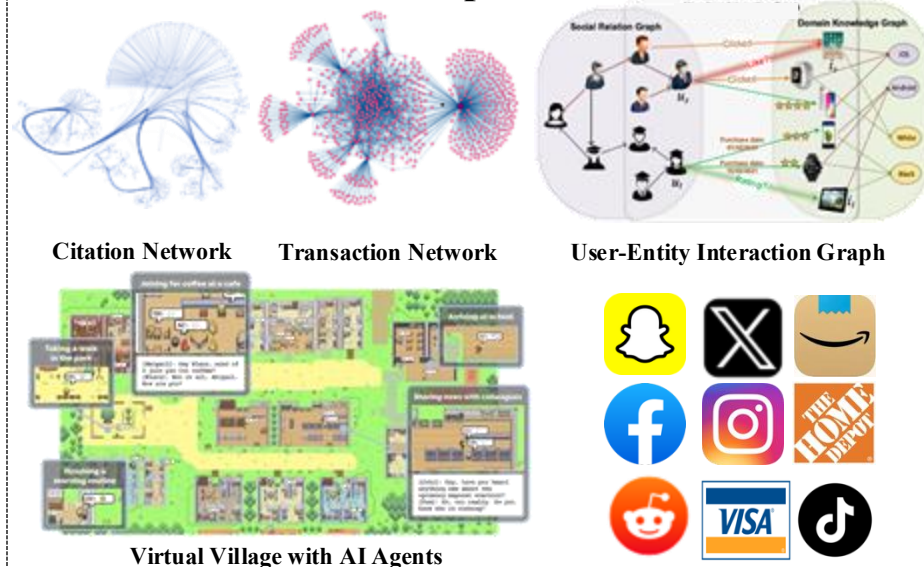
## Infrastructure Graph



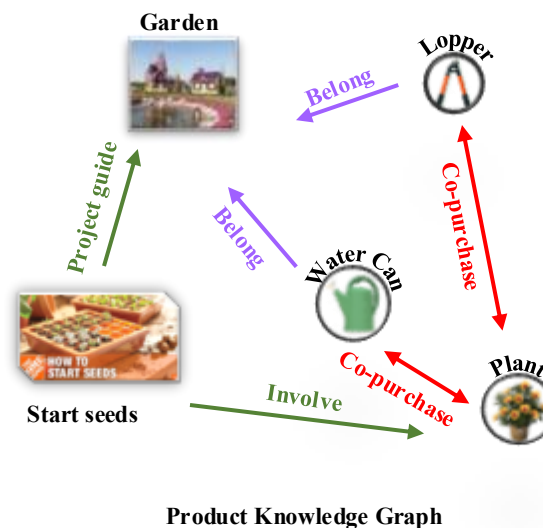
## Reasoning/Planning Graph



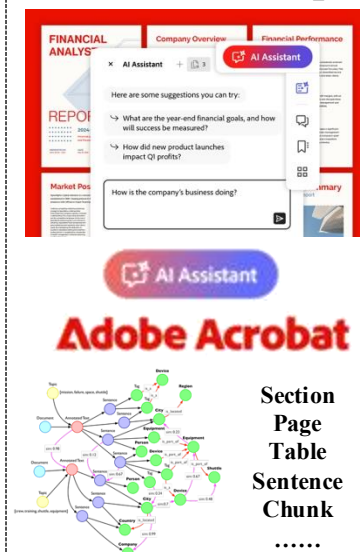
## Social Interaction Graph



## Knowledge Graph



## Document Graph





# Graph Retrieval-augmented Generation (GraphRAG)

Infrastructure Graph



Scene Graph



Tabular Graph



Biology Graph



Knowledge Graph



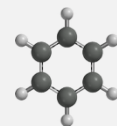
Document Graph



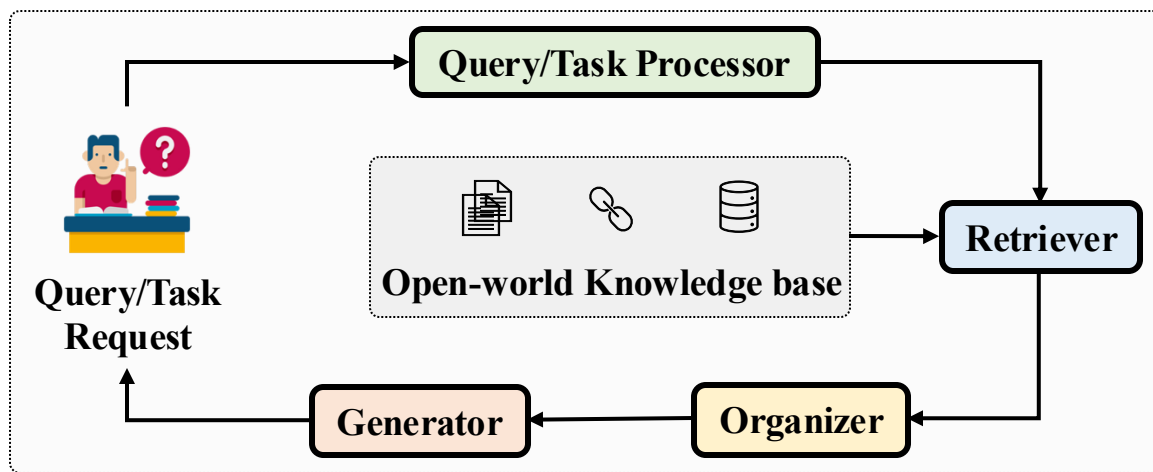
Social Graph



Scientific Graph



Reasoning Planning Graph



Name Entity Recognition

Relational Extraction

Query Structuration

Query Decomposition

Query Expansion

**Heuristic-**

Entity Linking

Relational Matching

Graph Traversal

Graph Kernel

Domain Expertise

**Learning-based**

Shallow Embedding

Deep Embedding

**Advanced**

Integrated

Iterative

Adaptive

**Reranking**

**Pruning**

Semantic-based

Syntactic-based

Structure-based

Dynamic

**Verbalization**

Linear-based

Template-based

**Augmentation**

Structure

Feature

**Prediction-based**

**LLM-based**

Verbalizing

Embedding-fusion

Positional Embedding-fusion

**Graph-based**

**Graph Construction**

Explicit Construction

Implicit Construction

# Graph Retrieval-augmented Generation (GraphRAG)

Infrastructure Graph



Scene Graph



Tabular Graph



Biology Graph



Knowledge Graph



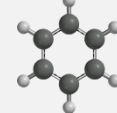
Document Graph



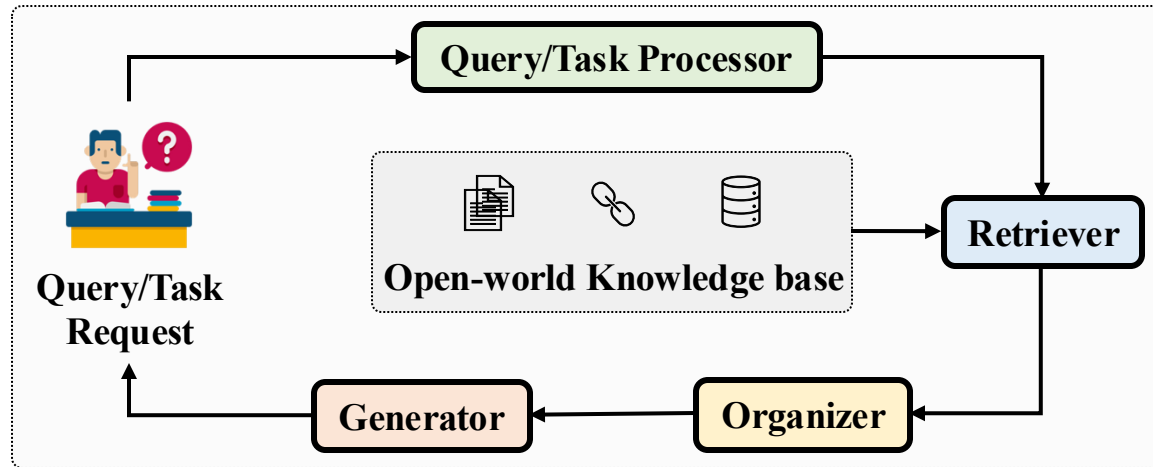
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Verbalizing

Embedding-fusion

Positional Embedding-fusion

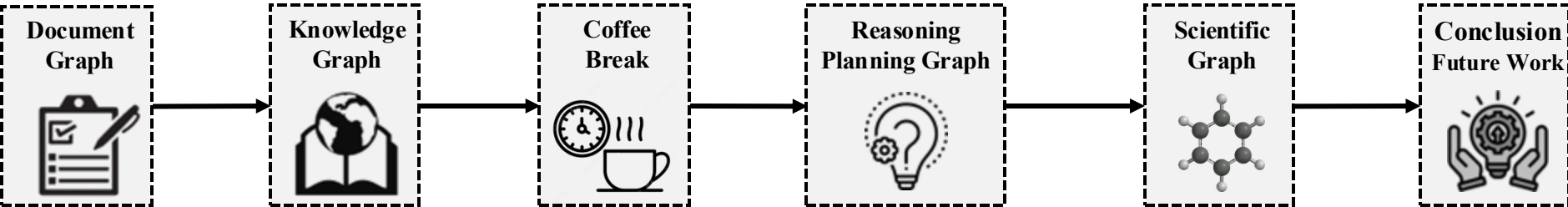
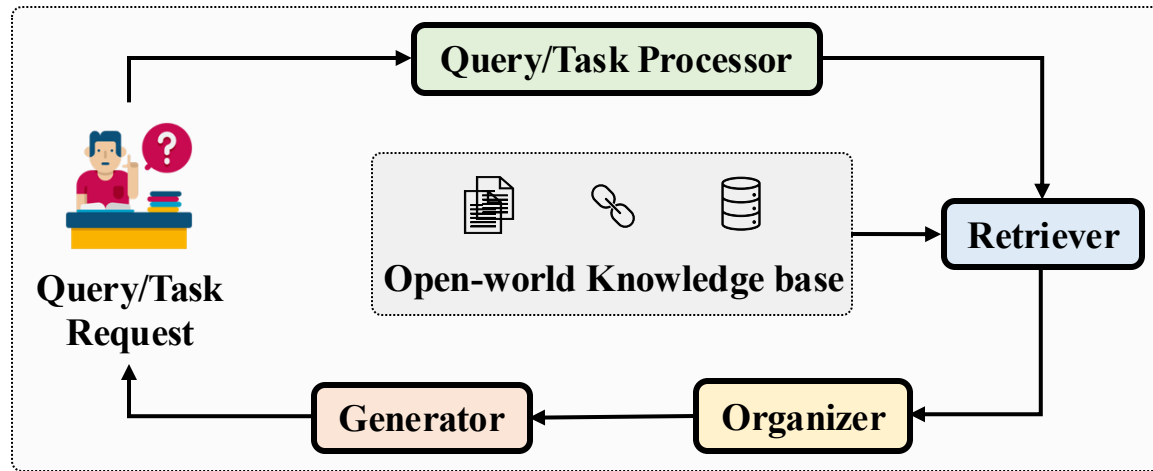
**Graph-based**

**Graph Construction**

Explicit Construction

Implicit Construction

# Outline



Haoyu Han  
24 min

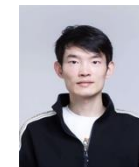


Harry Shomer  
24 min

4 min



Yongjia Lei  
24 min

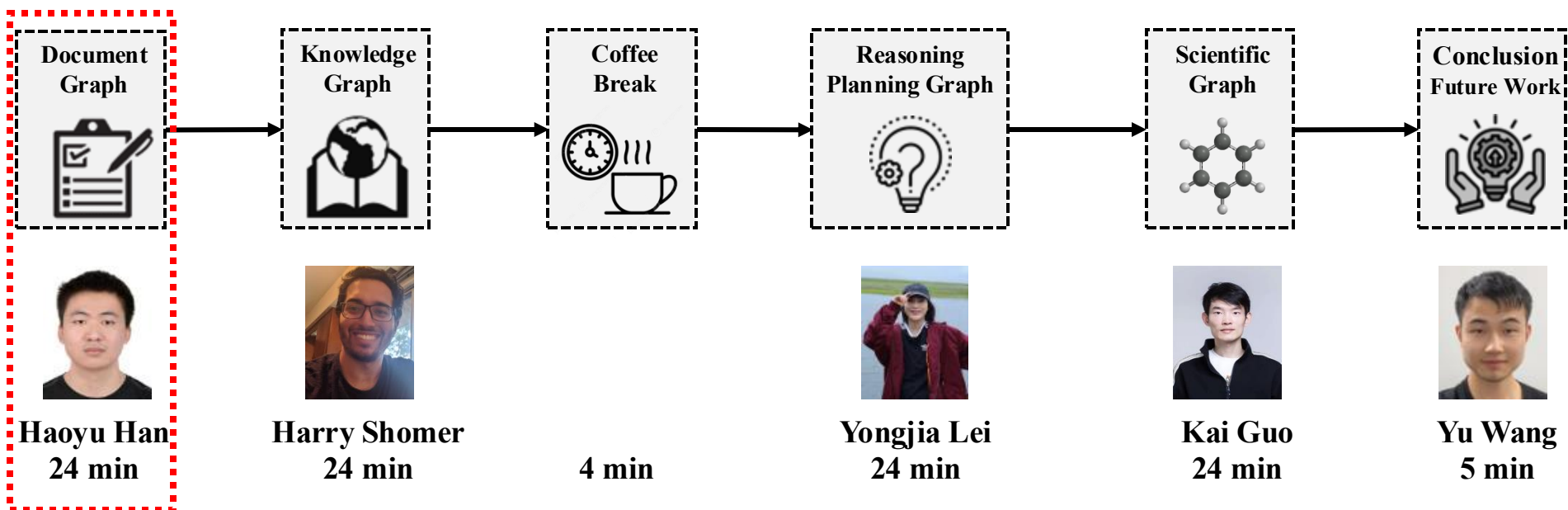
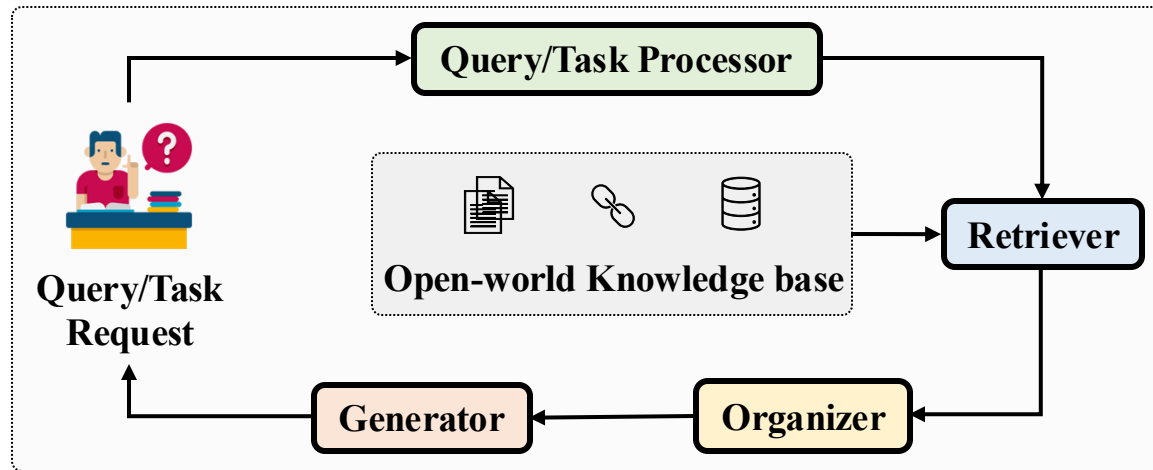


Kai Guo  
24 min



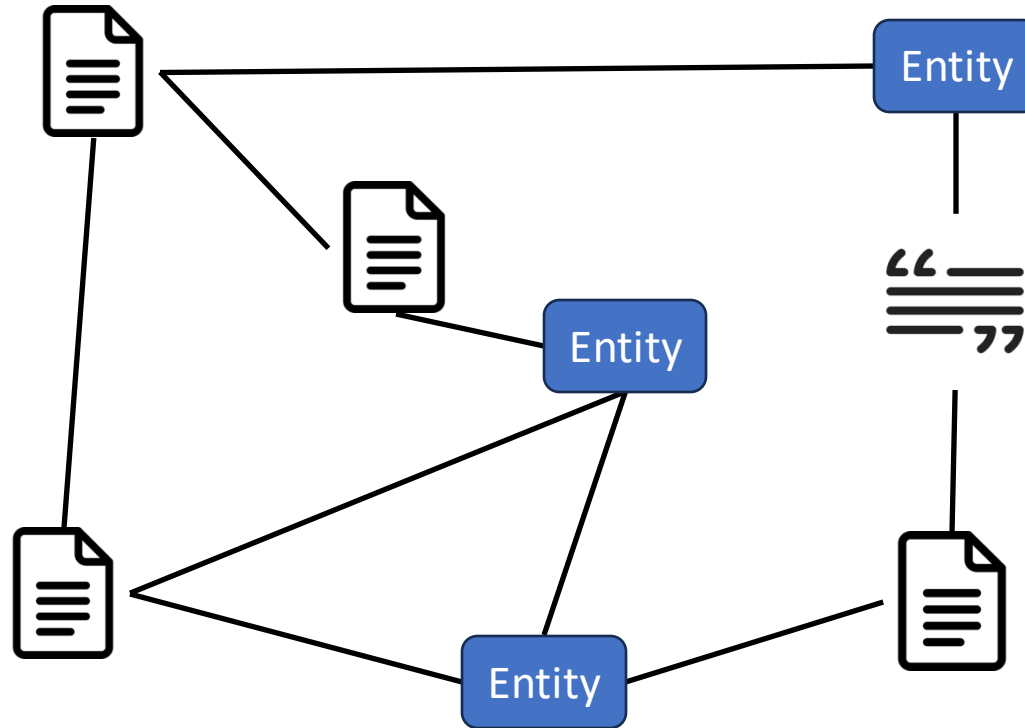
Yu Wang  
5 min

# Outline



# Document Graph

Connections between different documents or various granularity of documents.

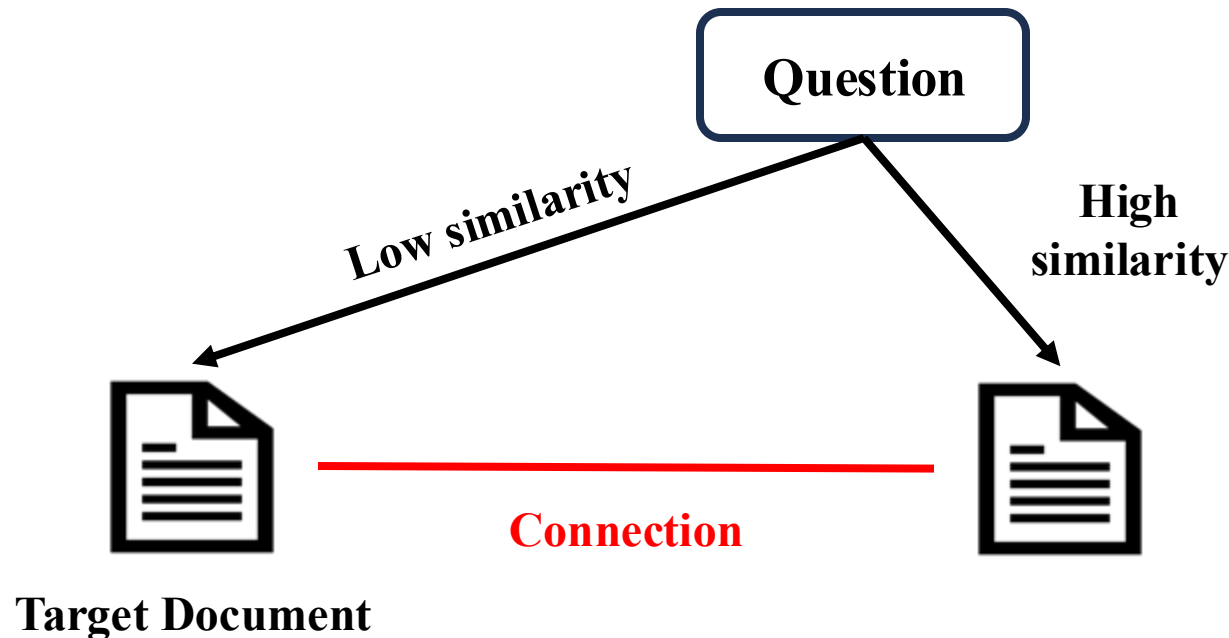


**Why should we build document graphs?**



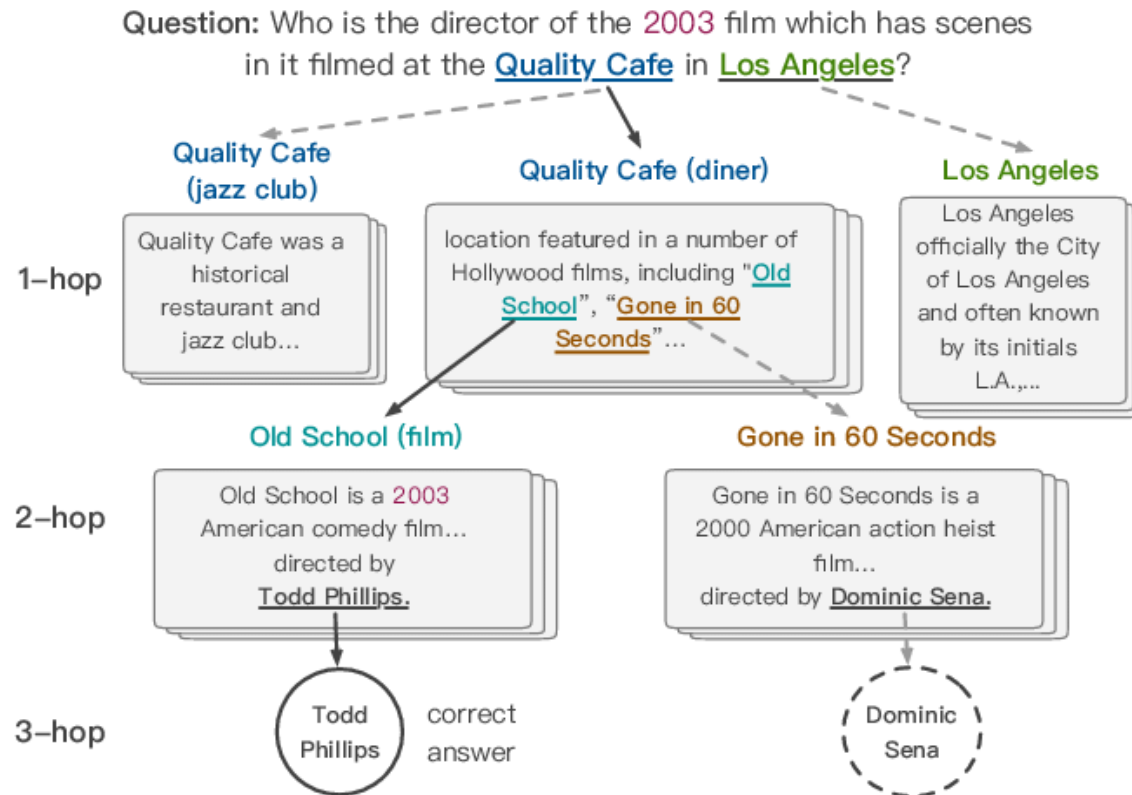
# Document Graph Motivation - Beyond Semantic Similarity

Target documents may have low similarity with the question.  
But can still be **retrieved via graph-based connections**.



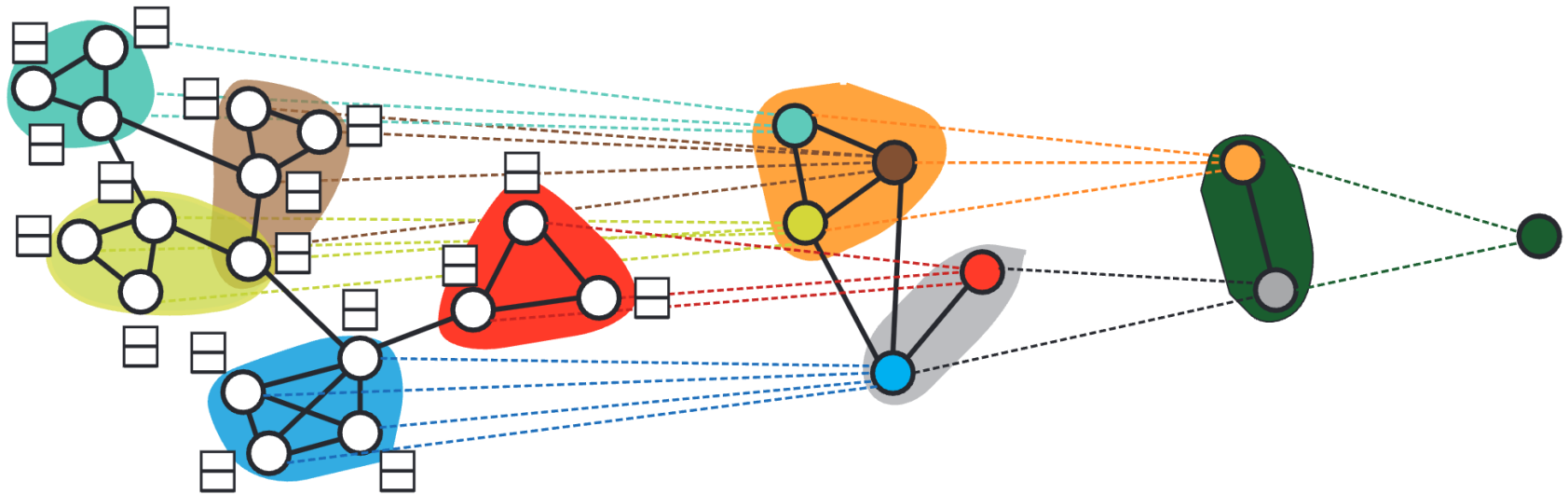
# Document Graph Motivation - Multi-hop Reasoning

The graph structure inherently supports multi-hop reasoning.



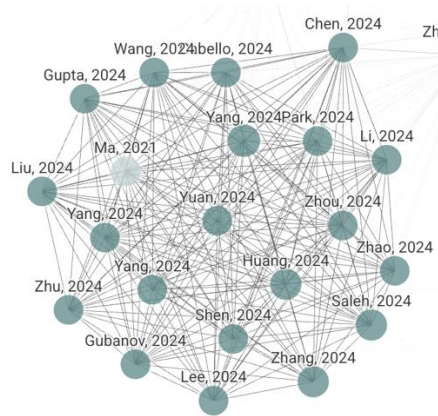
# Document Graph Motivation - Global Summarization

Hierarchical graph structure supports global information retrieval.

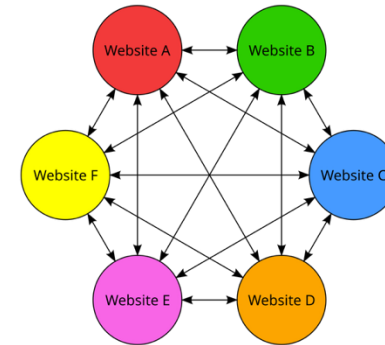


# Document Graph Construction – Explicit Construction

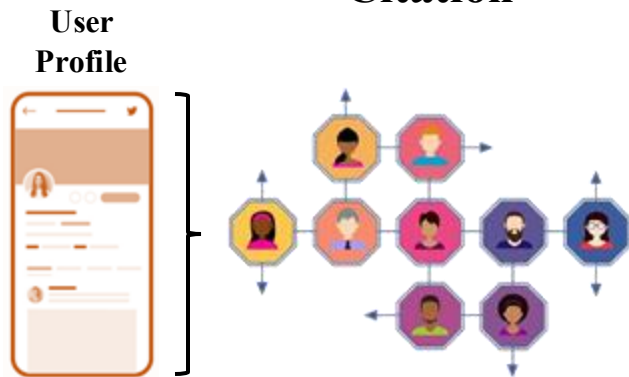
Building graphs using (pre)-defined relationships present in the data.



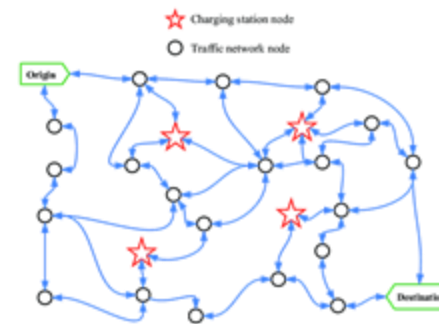
**Citation**



**Web Hyperlinks**



**Social Relation**



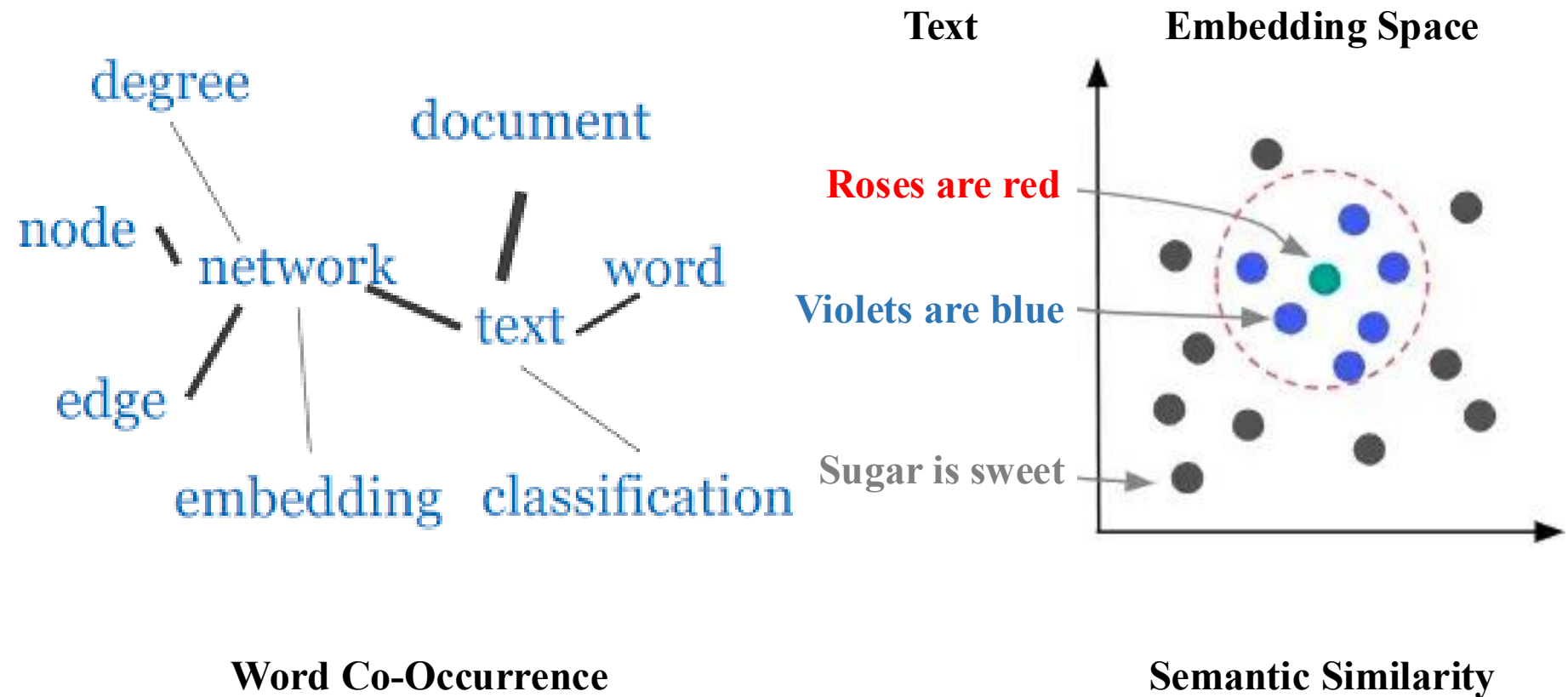
**Spatial Relation**

**Traffic Document**



# Document Graph Construction – Implicit Construction

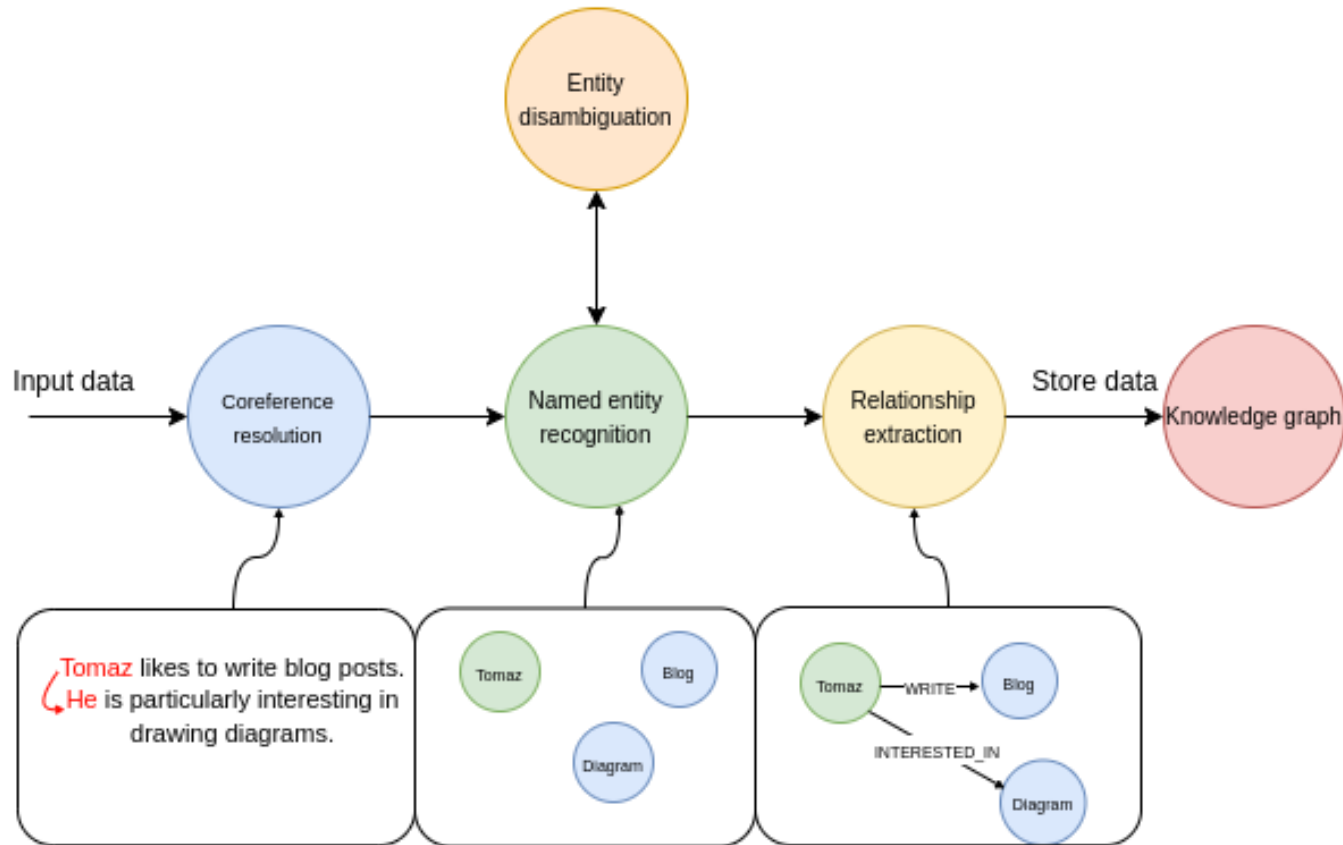
Building graphs by leveraging latent or implicit relations between nodes





# Document Graph Construction – Implicit Construction

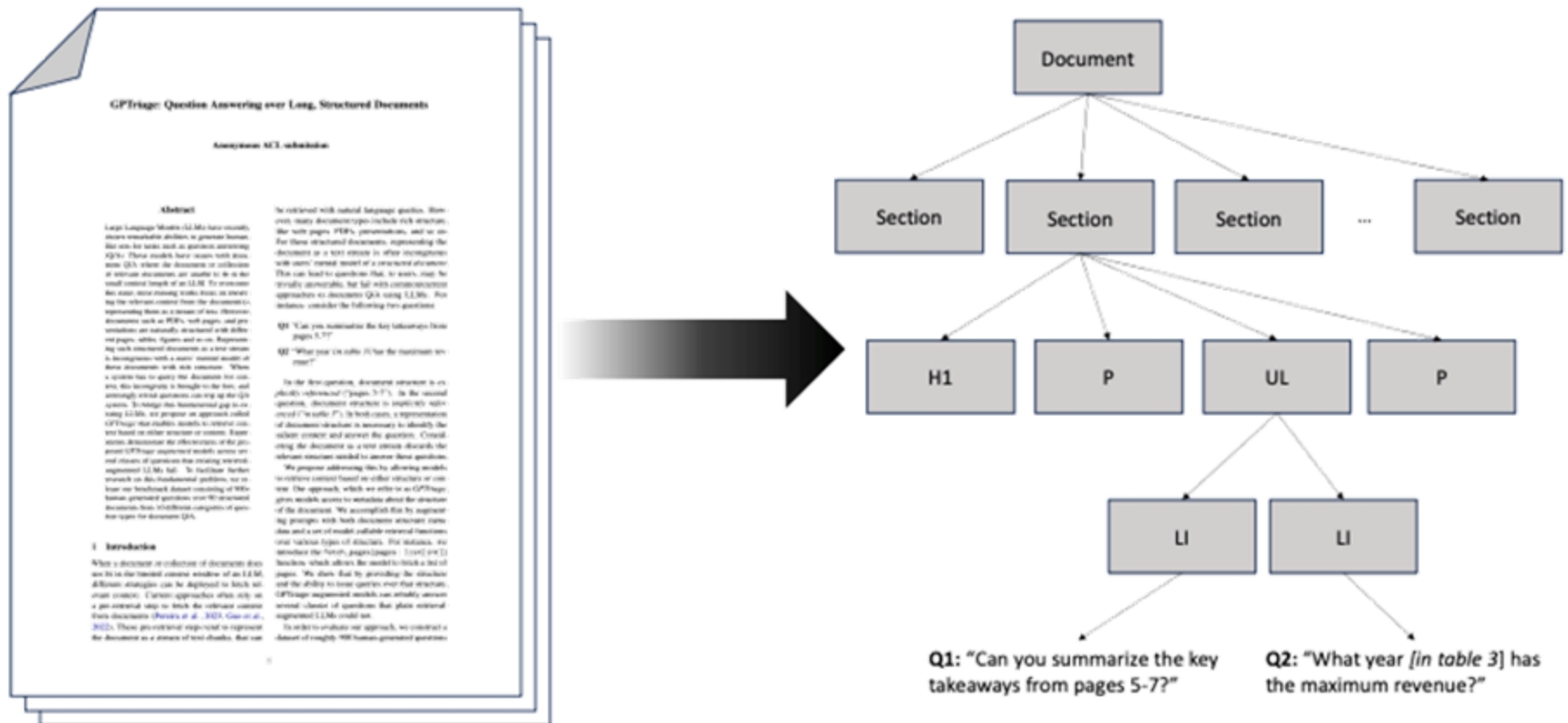
Building graphs by leveraging latent or implicit relations between nodes



**Entity and Relation Extraction**

# Document Graph Construction – Implicit Construction

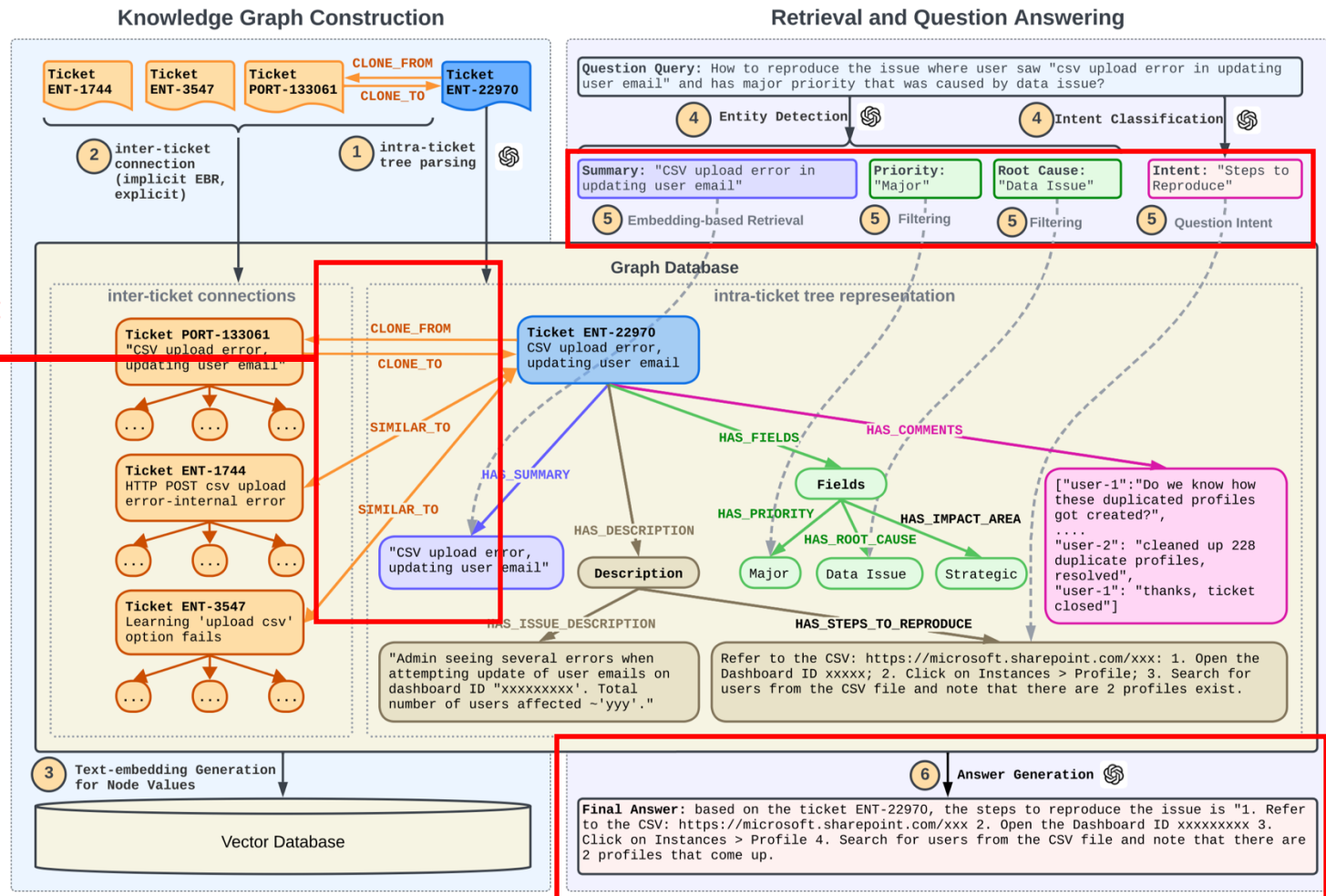
Building graphs by leveraging latent or implicit relations between nodes



## Document Structure

# Document Graph – Question-Answering

Leverage the solution of previous tickets to answer the current ticket



# Document Graph – Question-Answering

Leverage the solution of previous tickets to answer the current ticket

Table 1: Retrieval Performance

	MRR	Recall@K		NDCG@K	
		K=1	K=3	K=1	K=3
Baseline	0.522	0.400	0.640	0.400	0.520
Experiment	<b>0.927</b>	<b>0.860</b>	<b>1.000</b>	<b>0.860</b>	<b>0.946</b>

Table 2: Question Answering Performance

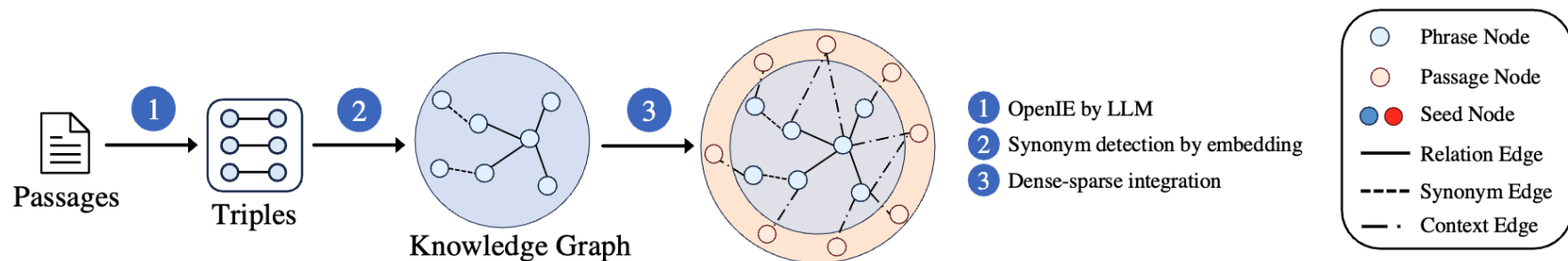
	BLEU	METEOR	ROUGE
Baseline	0.057	0.279	0.183
Experiment	<b>0.377</b>	<b>0.613</b>	<b>0.546</b>

Table 3: Customer Support Issue Resolution Time

Group	Mean	P50	P90
Tool Not Used	40 Hours	7 Hours	87 Hours
Tool Used	<b>15 hours</b>	<b>5 hours</b>	<b>47 hours</b>

# Document Graph – Question-Answering

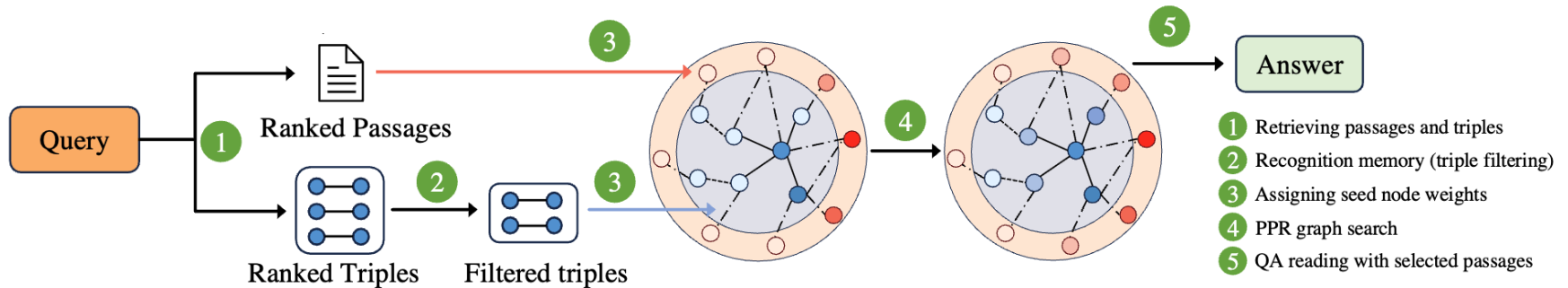
## HippoRAG 2 - Implicit graph construction from documents



1. Triplet Construction: LLMs extract entities/relations
2. Identify synonymous entities and connect them
3. Connect Extracted Entities with Originating Passages

# Document Graph – Question-Answering

## HippoRAG 2 - Retrieval & QA



1. Passage Retrieval by Semantic Similarity

2. Triplets-Retrieval

- Query Entity Extraction and map to the graph
- Similarity (Query, Nodes)
- Similarity (Query, Triplets)

3. Retrieve on the Graph: Personalized PageRank search

4. Answer Generation

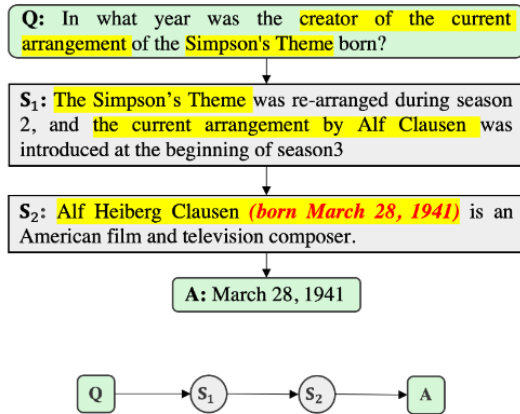
# Document Graph – Question-Answering

Retrieval	Simple QA		Multi-Hop QA				Discourse Understanding	Avg
	NQ	PopQA	MuSiQue	2Wiki	HotpotQA	LV-Eval	NarrativeQA	
Simple Baselines								
None	54.9	32.5	26.1	42.8	47.3	6.0	12.9	38.4
Contriever (Izacard et al., 2022)	58.9	53.1	31.3	41.9	62.3	8.1	19.7	46.9
BM25 (Robertson & Walker, 1994)	59.0	49.9	28.8	51.2	63.4	5.9	18.3	47.7
GTR (T5-base) (Ni et al., 2022)	59.9	56.2	34.6	52.8	62.8	7.1	19.9	50.4
Large Embedding Models								
GTE-Qwen2-7B-Instruct (Li et al., 2023)	62.0	56.3	40.9	60.0	71.0	7.1	21.3	54.9
GritLM-7B (Muennighoff et al., 2024)	61.3	55.8	44.8	60.6	73.3	9.8	23.9	56.1
NV-Embed-v2 (7B) (Lee et al., 2025)	61.9	55.7	45.7	61.5	75.3	9.8	25.7	57.0
Structure-Augmented RAG								
RAPTOR (Sarathi et al., 2024)	50.7	56.2	28.9	52.1	69.5	5.0	21.4	48.8
GraphRAG (Edge et al., 2024)	46.9	48.1	38.5	58.6	68.6	11.2	23.0	49.6
LightRAG (Guo et al., 2024)	16.6	2.4	1.6	11.6	2.4	1.0	3.7	6.6
HippoRAG (Gutiérrez et al., 2024)	55.3	55.9	35.1	71.8	63.5	8.4	16.3	53.1
HippoRAG 2	63.3	56.2	48.6	71.0	75.5	12.9	25.9	59.8

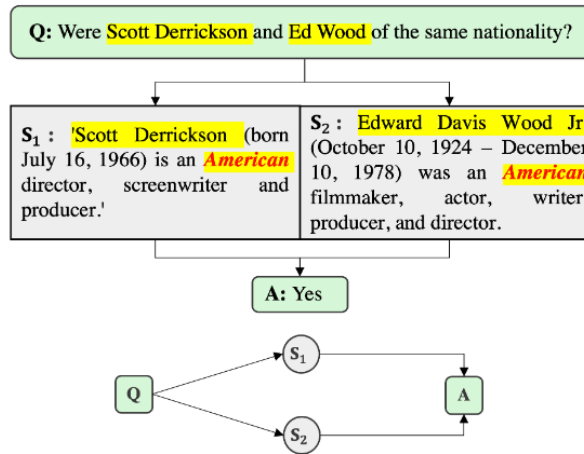
**GraphRAG is typically more effective for multi-hop QA.**

# Document Graph – Question-Answering

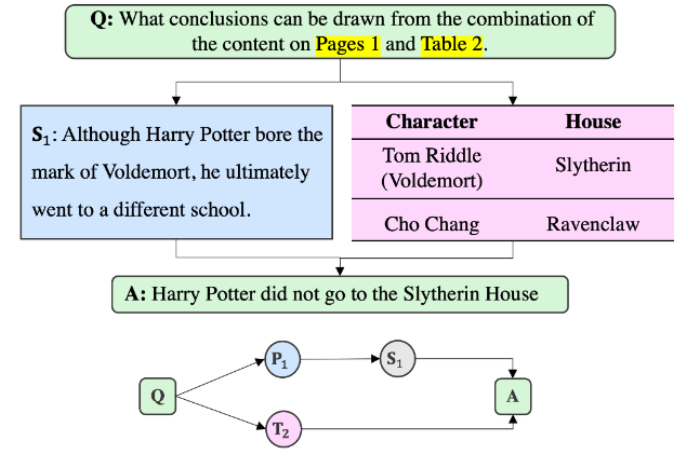
(a) Content question - Bridging



(b) Content question - Comparing



(c) Structural question



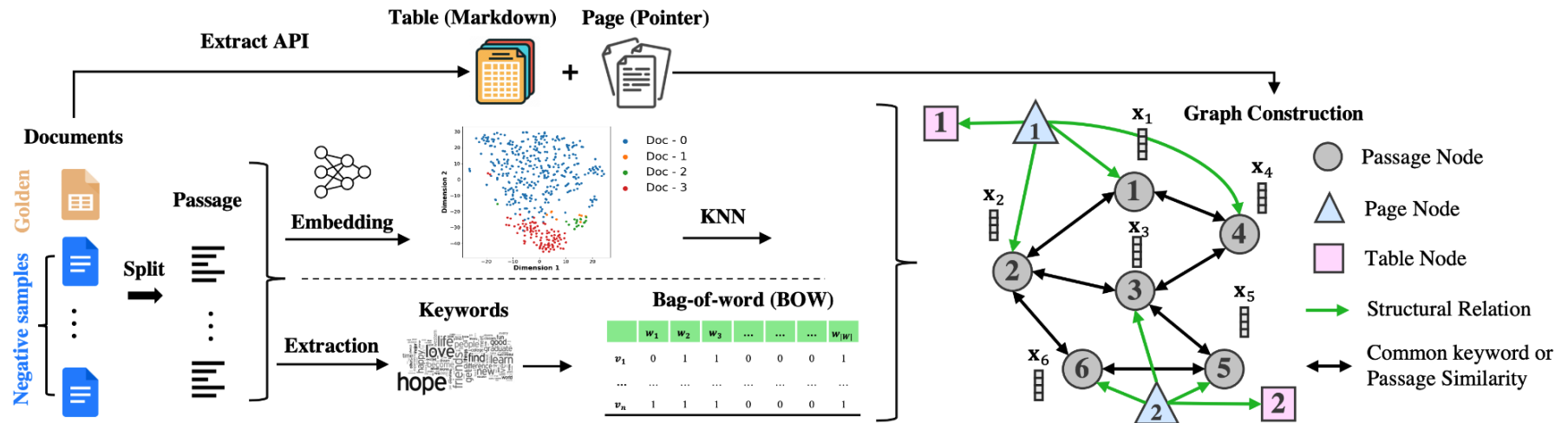
Lexical similarity

Semantic similarity

Document Structure



# Document Graph – Question-Answering



## 1. Graph Construction

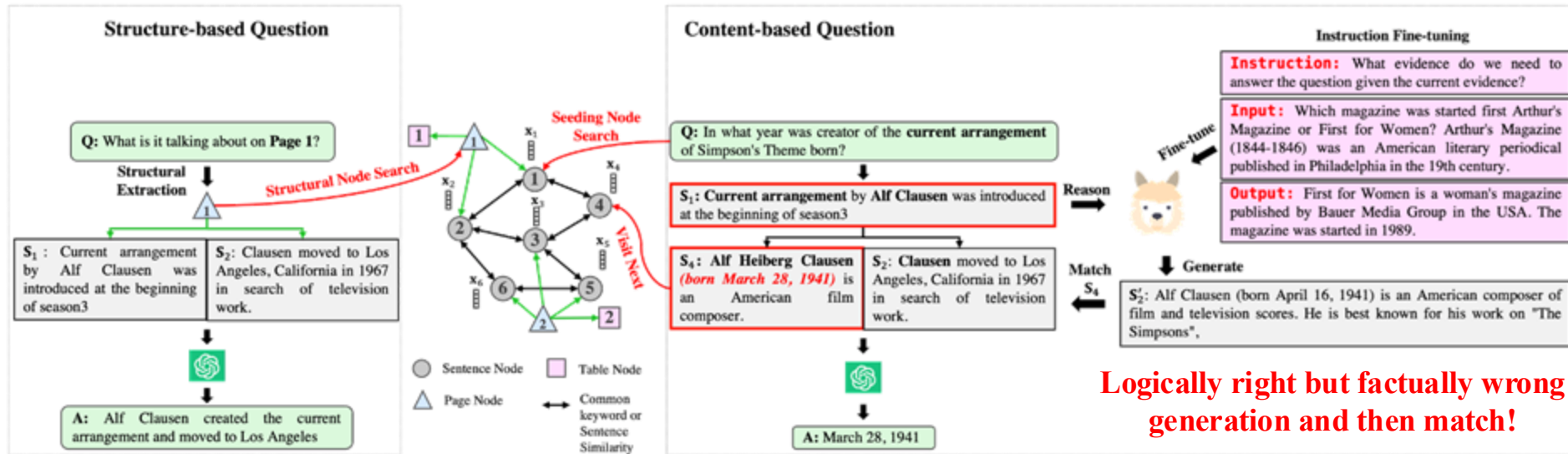
a. TF-IDF construction

b. KNN construction

c. Connect passages share same entity

d. Add Table/Page Document Meta-Structure

# Document Graph – Question-Answering



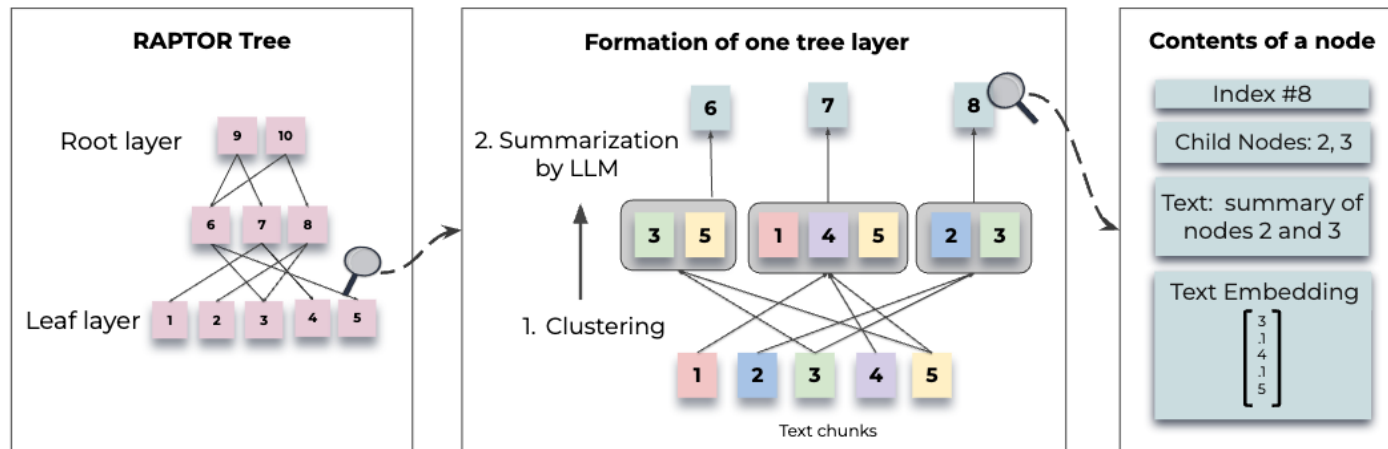
## 2. Retrieval (LLM traversal agent for reasoning and grounding)

- Initialize the seeding passage with similarity search
- LLMs predict the next passage to explore
- Retrieve passages based on LLM's generation

# Document Graph – Question-Answering

## RAPTOR – Tree-based Retrieval

Tree structure to capture **High/Low-level** information



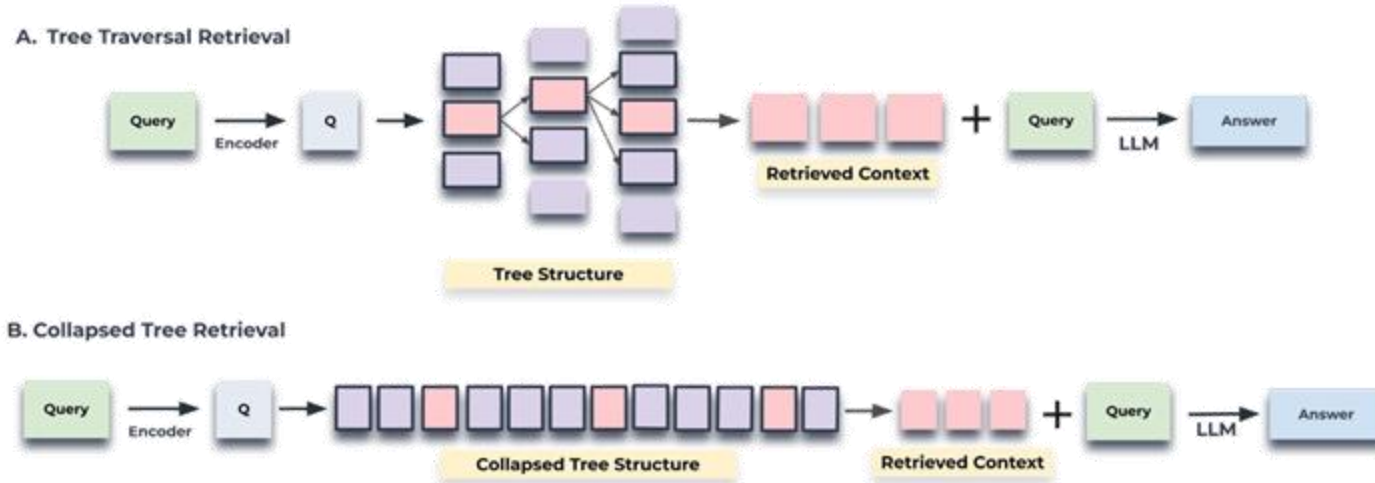
### 1. Graph Construction

- Represent each leaf node as a text chunk
- Apply clustering algorithms to group related chunks
- Summarize each cluster to form higher-level nodes
- Repeat the construction process

# Document Graph – Question-Answering

## RAPTOR – Tree-based Retrieval

Tree structure to capture **High/Low-level** information



## 2. Retrieval

- Tree Traversal Retrieval: Root-to-Leaf Traversal, Progressively Narrowing Down
- Collapsed Tree Retrieval: Flatten Tree Structure, Independently Retrieve

# Document Graph – Question-Answering

## RAPTOR – Tree-based Retrieval

Tree structure to capture **High/Low-level** information

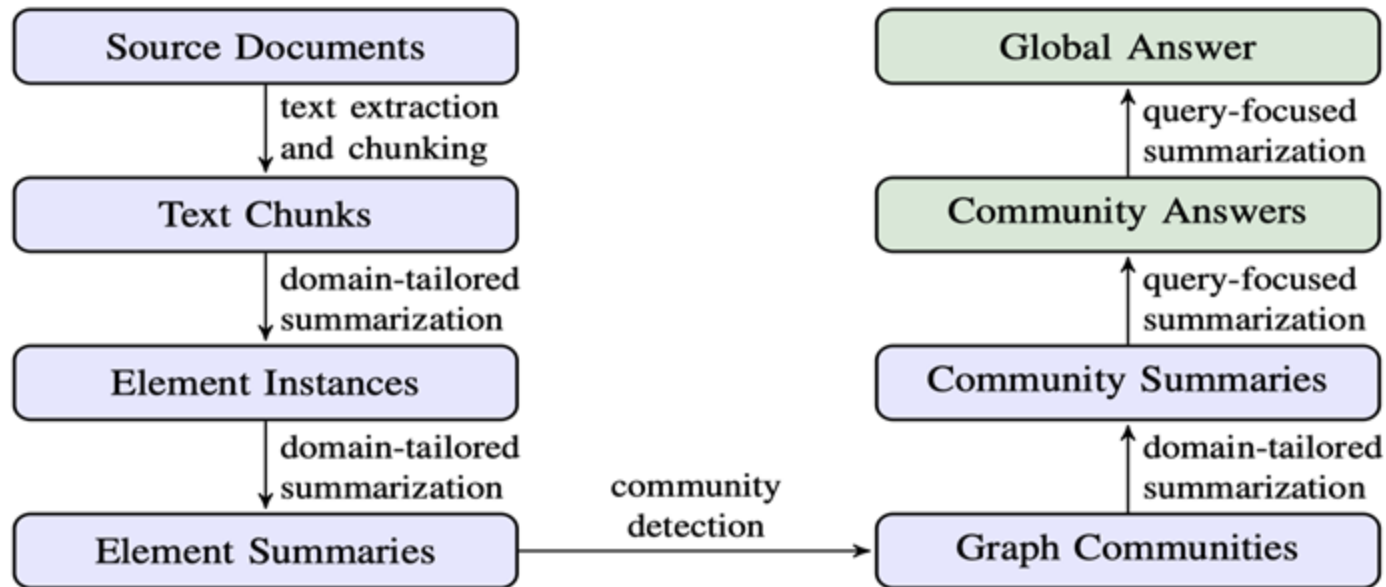
Model	ROUGE	BLEU-1	BLEU-4	METEOR
<b>SBERT with RAPTOR</b>	<b>30.87%</b>	<b>23.50%</b>	<b>6.42%</b>	<b>19.20%</b>
SBERT without RAPTOR	29.26%	22.56%	5.95%	18.15%
<b>BM25 with RAPTOR</b>	<b>27.93%</b>	<b>21.17%</b>	<b>5.70%</b>	<b>17.03%</b>
BM25 without RAPTOR	23.52%	17.73%	4.65%	13.98%
<b>DPR with RAPTOR</b>	<b>30.94%</b>	<b>23.51%</b>	<b>6.45%</b>	<b>19.05%</b>
DPR without RAPTOR	29.56%	22.84%	6.12%	18.44%

**Tree-based retrieval improves global QA performance.**

# Document Graph – Document Summarization

## Microsoft GraphRAG

Corpus to summarize too large      vs      LLM context window is limited

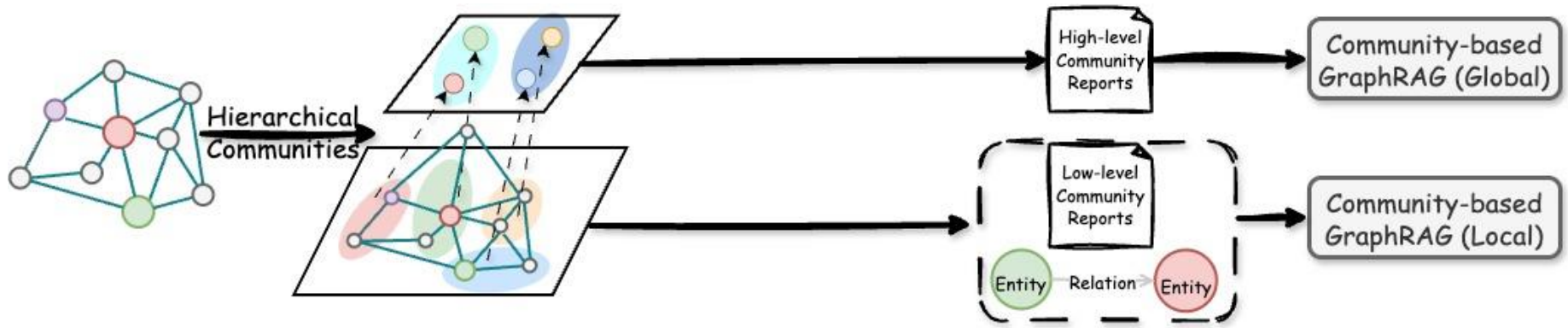


Extract a knowledge graph  
from the whole corpus.

Hierarchical Community  
Detection and Summarization  
Multiple Granularities

# Document Graph – Document Summarization

## Microsoft GraphRAG



1. **Local Retrieval** from leaf nodes
2. **Global Retrieval** from summarization nodes

# Document Graph – Document Summarization

## Microsoft GraphRAG

### Podcast transcripts

	SS	TS	C0	C1	C2	C3
SS	50	17	28	25	22	21
TS	83	50	50	48	43	44
C0	72	50	50	53	50	49
C1	75	52	47	50	52	50
C2	78	57	50	48	50	52
C3	79	56	51	50	48	50

Comprehensiveness

	SS	TS	C0	C1	C2	C3
SS	50	18	23	25	19	19
TS	82	50	50	50	43	46
C0	77	50	50	50	46	44
C1	75	50	50	50	44	45
C2	81	57	54	56	50	48
C3	81	54	56	55	52	50

Diversity

	SS	TS	C0	C1	C2	C3
SS	50	42	57	52	49	51
TS	58	50	59	55	52	51
C0	43	41	50	49	47	48
C1	48	45	51	50	49	50
C2	51	48	53	51	50	51
C3	49	49	52	50	49	50

Empowerment

	SS	TS	C0	C1	C2	C3
SS	50	56	65	60	60	60
TS	44	50	55	52	51	52
C0	35	45	50	47	48	48
C1	40	48	53	50	50	50
C2	40	49	52	50	50	50
C3	40	48	52	50	50	50

Directness

### News articles

	SS	TS	C0	C1	C2	C3
SS	50	20	28	25	21	21
TS	80	50	44	41	38	36
C0	72	56	50	52	54	52
C1	75	59	48	50	58	55
C2	79	62	46	42	50	59
C3	79	64	48	45	41	50

Comprehensiveness

	SS	TS	C0	C1	C2	C3
SS	50	33	38	35	29	31
TS	67	50	53	45	44	40
C0	62	47	50	40	41	41
C1	65	55	60	50	50	50
C2	71	56	59	50	50	51
C3	69	60	59	50	49	50

Diversity

	SS	TS	C0	C1	C2	C3
SS	50	47	57	49	50	50
TS	53	50	58	50	50	48
C0	43	42	50	42	45	44
C1	51	50	58	50	52	51
C2	50	50	55	48	50	50
C3	50	52	56	49	50	50

Empowerment

	SS	TS	C0	C1	C2	C3
SS	50	54	59	55	55	54
TS	46	50	55	53	52	52
C0	41	45	50	48	48	47
C1	45	47	52	50	49	49
C2	45	48	52	51	50	49
C3	46	48	53	51	51	50

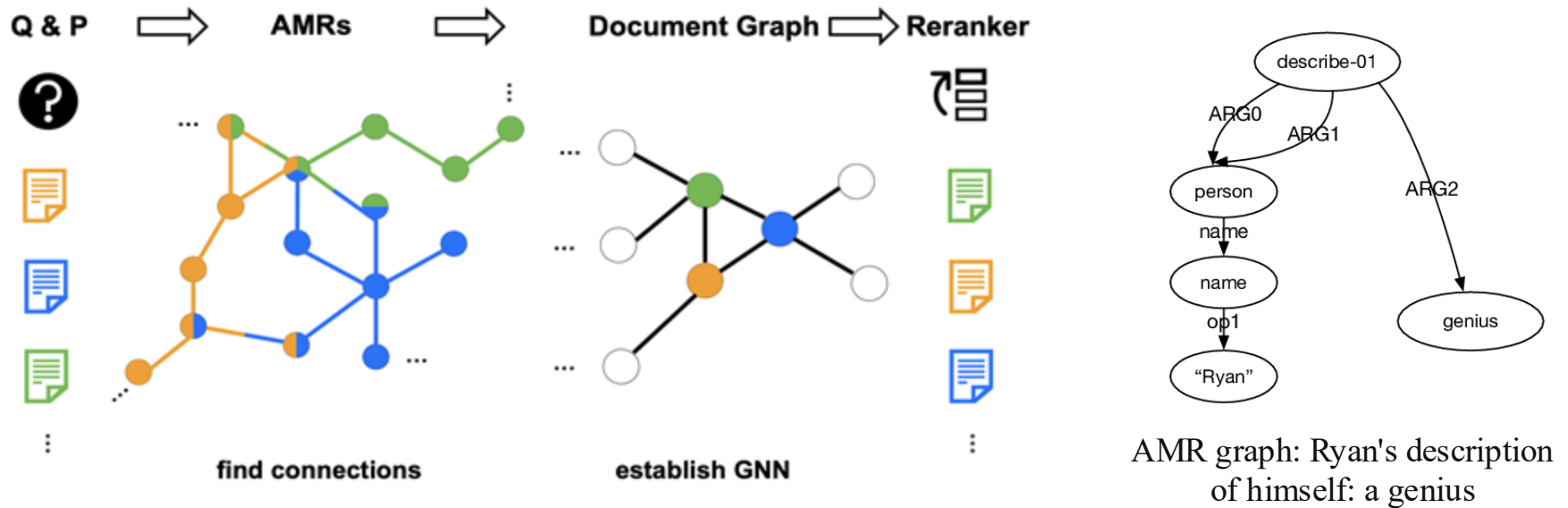
Directness

**GraphRAG is typically superior in both comprehensiveness and diversity.**



# Document Graph – Document Retrieval

## G-RAG : A document-graph-based reranker



### 1. Graph Construction

- Build Abstract Meaning Representation (AMR) graphs
- Connect documents share same nodes

# Document Graph – Document Retrieval

## G-RAG : A document-graph-based reranker

### 2. GNNs for Reranking

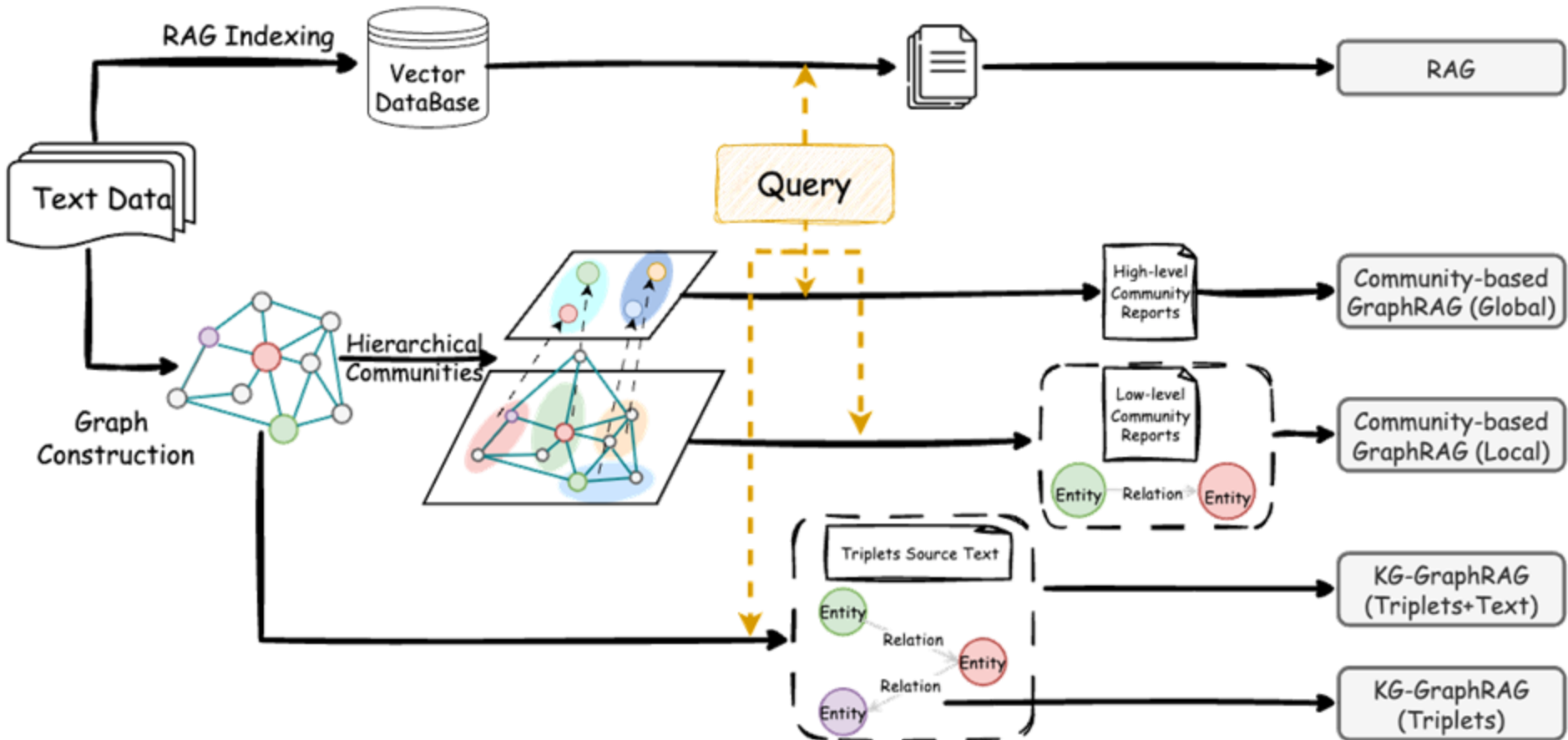
Document and query embedding:  $\mathbf{x}_v^\ell = g\left(\mathbf{x}_v^{\ell-1}, \bigcup_{u \in \mathcal{N}(v)} f(\mathbf{x}_u^{\ell-1}, \mathbf{e}_{uv}^{\ell-1})\right) \quad \mathbf{y} = \text{Encode}(q).$

Ranking based on the similarity:  $s_i = \mathbf{y}^\top \mathbf{x}_{v_i}^L$

Ranking loss  $\mathcal{RL}_q(s_i, s_j, r) = \max(0, -r(s_i - s_j) + 1),$

# RAG vs. GraphRAG

A systematic evaluation between RAG and GraphRAG.



# RAG vs. GraphRAG: QA Task

## Single-Hop

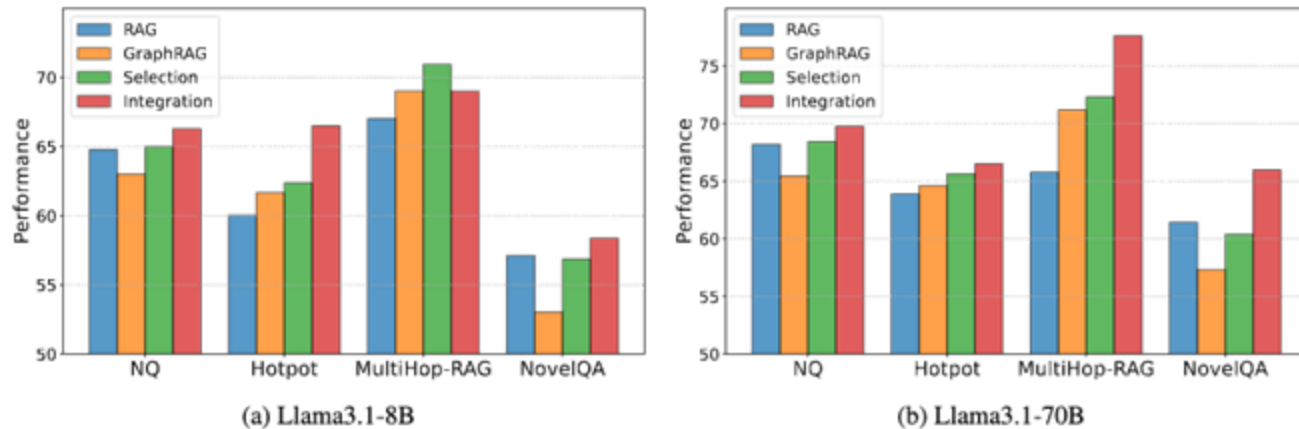
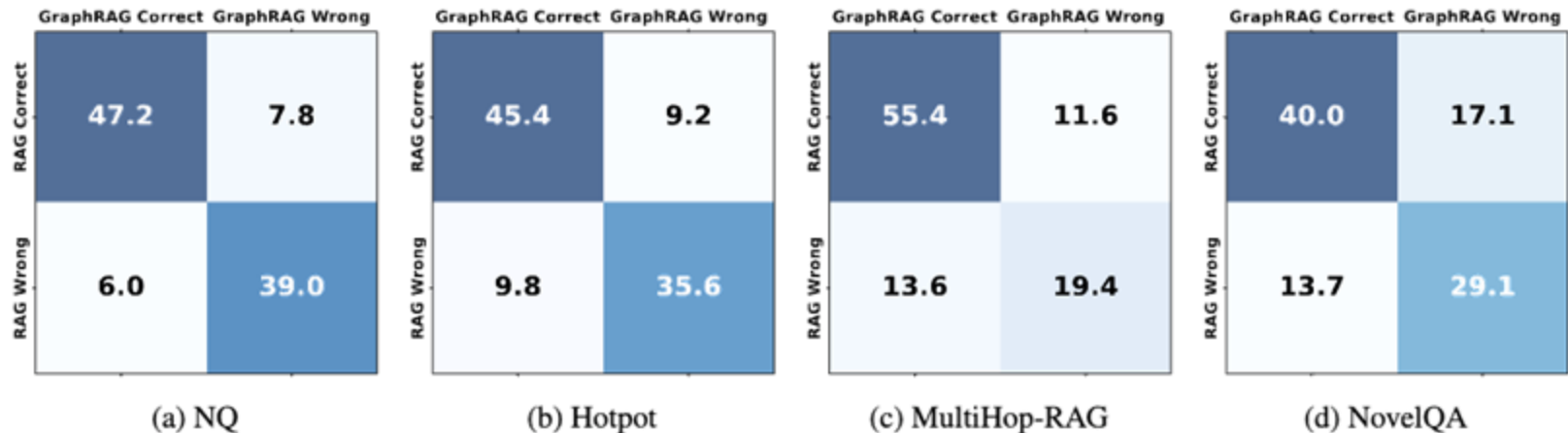
## Multi-Hop

Method	NQ						Hotpot					
	Llama 3.1-8B			Llama 3.1-70B			Llama 3.1-8B			Llama 3.1-70B		
	P	R	F1	P	R	F1	P	R	F1	P	R	F1
RAG	<b>71.7</b>	<b>63.93</b>	<b>64.78</b>	<b>74.55</b>	<b>67.82</b>	<b>68.18</b>	<u>62.32</u>	<u>60.47</u>	<u>60.04</u>	<u>66.34</u>	<u>63.99</u>	<u>63.88</u>
KG-GraphRAG (Triplets only)	40.09	33.56	34.28	37.84	31.22	28.50	26.88	24.81	25.02	32.59	30.63	30.73
KG-GraphRAG (Triplets+Text)	58.36	48.93	50.27	60.91	52.75	53.88	45.22	42.85	42.60	51.44	48.99	48.75
Community-GraphRAG (Local)	<u>69.48</u>	<u>62.54</u>	<u>63.01</u>	<u>71.27</u>	<u>65.46</u>	<u>65.44</u>	<b>64.14</b>	<b>62.08</b>	<b>61.66</b>	<b>67.20</b>	<b>64.89</b>	<b>64.60</b>
Community-GraphRAG (Global)	60.76	54.99	54.48	61.15	55.52	55.05	45.72	47.60	45.16	48.33	48.56	46.99

- RAG excels on detailed single-hop queries.
- GraphRAG, particularly CommunityGraphRAG (Local), excels on multi-hop queries.
- Community-GraphRAG (Global) often struggles on QA tasks.
- KG-based GraphRAG also generally underperform on QA tasks due to the incomplete graph.

# RAG vs. GraphRAG: QA Task

**RAG and GraphRAG are Complementary!**



**Combining RAG and GraphRAG yields better performance!**

# RAG vs. GraphRAG: Summarization Task

## Ground Truth (Human Answer) as Judge

Table 4: The performance of query-based single document summarization task using Llama3.1-8B.

Method	SQuALITY						QMSum					
	ROUGE-2			BERTScore			ROUGE-2			BERTScore		
	P	R	F1	P	R	F1	P	R	F1	P	R	F1
RAG	15.09	8.74	10.08	74.54	81.00	77.62	<u>21.50</u>	<b>3.80</b>	<u>6.32</u>	<b>81.03</b>	<u>84.45</u>	<b>82.69</b>
KG-GraphRAG (Triplets only)	11.99	6.16	7.41	82.46	84.30	83.17	13.71	2.55	4.15	80.16	82.96	81.52
KG-GraphRAG (Triplets+Text)	15.00	<b>9.48</b>	<u>10.52</u>	<b>84.37</b>	<b>85.88</b>	<b>84.92</b>	16.83	3.32	5.38	<u>80.92</u>	83.64	82.25
Community-GraphRAG (Local)	<b>15.82</b>	8.64	10.10	<u>83.93</u>	85.84	84.66	20.54	3.35	5.64	80.63	84.13	82.34
Community-GraphRAG (Global)	10.23	6.21	6.99	82.68	84.26	83.30	10.54	1.97	3.23	79.79	82.47	81.10
Integration	<u>15.69</u>	<u>9.32</u>	<b>10.67</b>	74.56	81.22	77.73	<b>21.97</b>	<b>3.80</b>	<b>6.34</b>	80.89	<b>84.47</b>	<u>82.63</u>

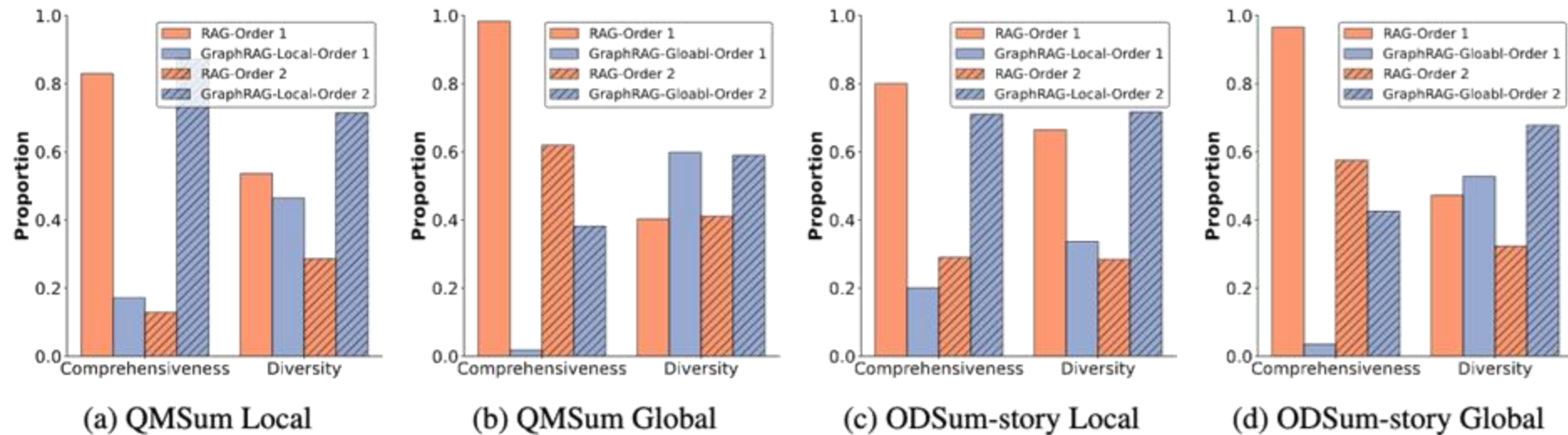
Table 5: The performance of query-based multiple document summarization task using Llama3.1-8B.

Method	ODSum-story						ODSum-meeting					
	ROUGE-2			BERTScore			ROUGE-2			BERTScore		
	P	R	F1	P	R	F1	P	R	F1	P	R	F1
RAG	<b>15.39</b>	<u>8.44</u>	<b>9.81</b>	<b>83.87</b>	<b>85.74</b>	<b>84.57</b>	15.50	<b>6.43</b>	<b>8.77</b>	<b>83.12</b>	<b>85.84</b>	<b>84.45</b>
KG-GraphRAG (Triplets only)	11.02	5.56	6.62	82.09	83.91	82.77	11.64	4.87	6.58	81.13	84.32	82.69
KG-GraphRAG (Triplets+Text)	9.19	5.82	6.22	79.39	83.30	81.03	11.97	4.97	6.72	81.50	84.41	82.92
Community-GraphRAG (Local)	<u>13.84</u>	7.19	8.49	83.19	85.07	83.90	<u>15.65</u>	5.66	8.02	82.44	85.54	83.96
Community-GraphRAG (Global)	9.40	4.47	5.46	81.46	83.54	82.30	11.44	3.89	5.59	81.20	84.50	82.81
Integration	14.77	<b>8.55</b>	<u>9.53</u>	<u>83.73</u>	<u>85.56</u>	<u>84.40</u>	<b>15.69</b>	<u>6.15</u>	<u>8.51</u>	<u>82.87</u>	<u>85.81</u>	<u>84.31</u>

**RAG aligns more closely with human-written answers.**

# RAG vs. GraphRAG: Summarization Task

## LLM as Judge



1. Strong position bias is observed
2. Community-based GraphRAG with global search prefers corpus global structure

# Document Graph - Future Works

## 1. Graph Construction

- a. Task-specific graph construction
- b. Balancing efficiency and graph completeness

## 2. Retrieval and Traversal

- a. Adaptive retrieval strategies based on query type and complexity
- b. Multi-hop retrieval with reasoning over graph structure

## 3. RAG and GraphRAG Integration

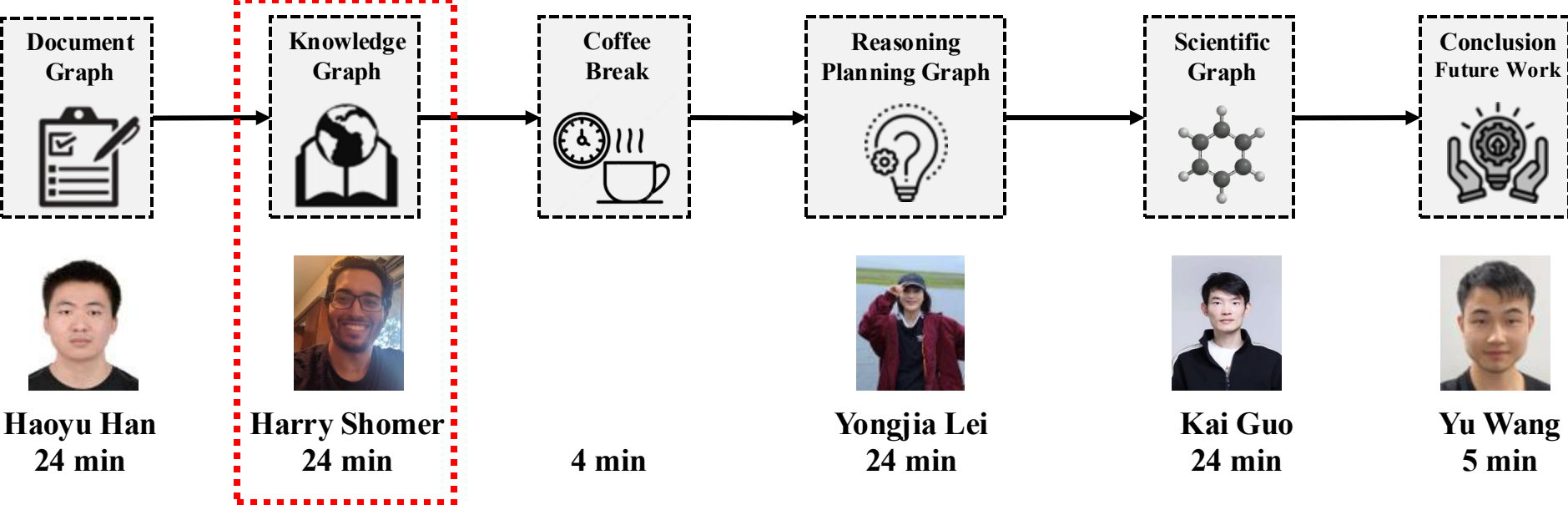
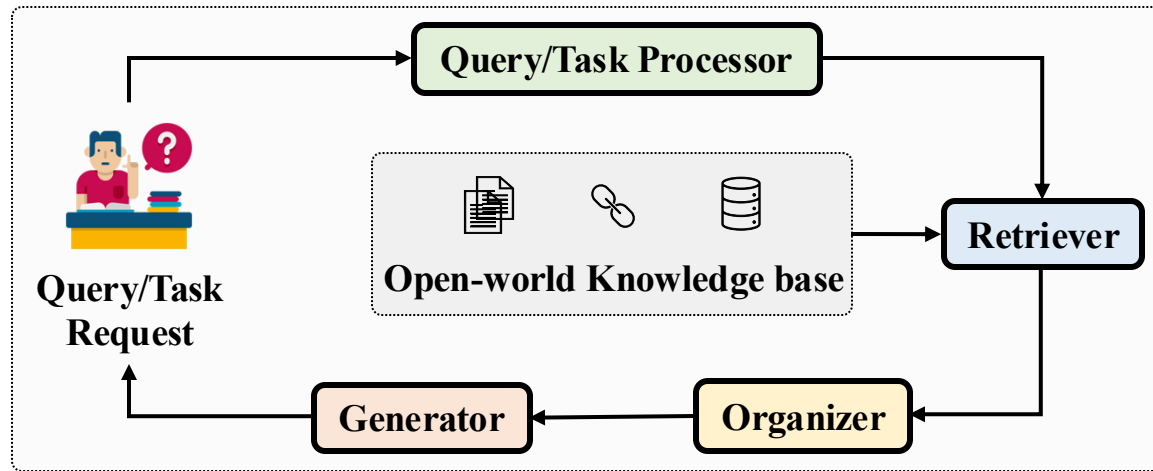
- a. Analyzing the Pros and Cons of RAG and GraphRAG
- b. Designing methods to combine their strengths

## 4. Evaluation

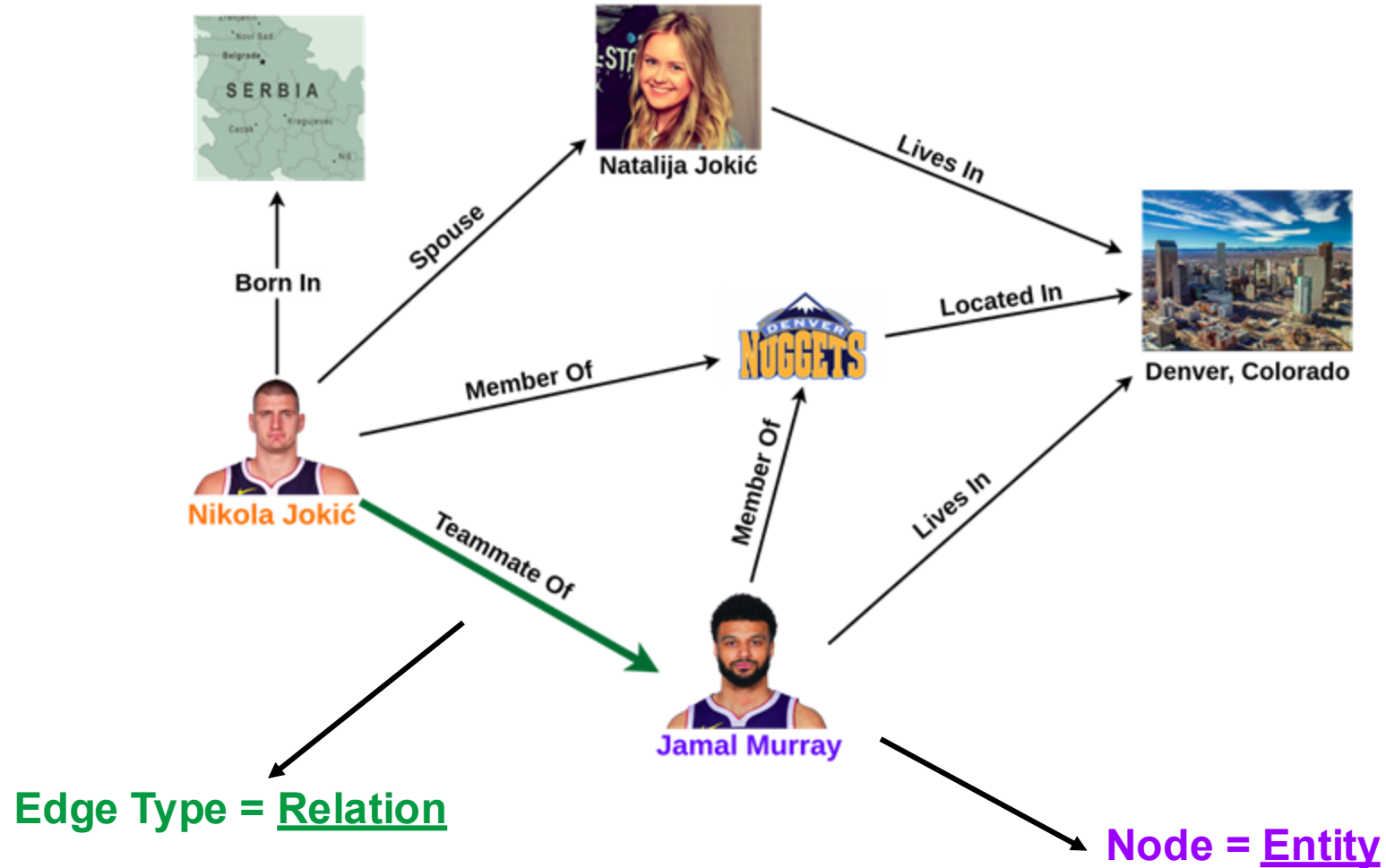
- a. New benchmarks designed specifically for graph-based retrieval and generation
- b. Proposing fine-grained evaluation metrics



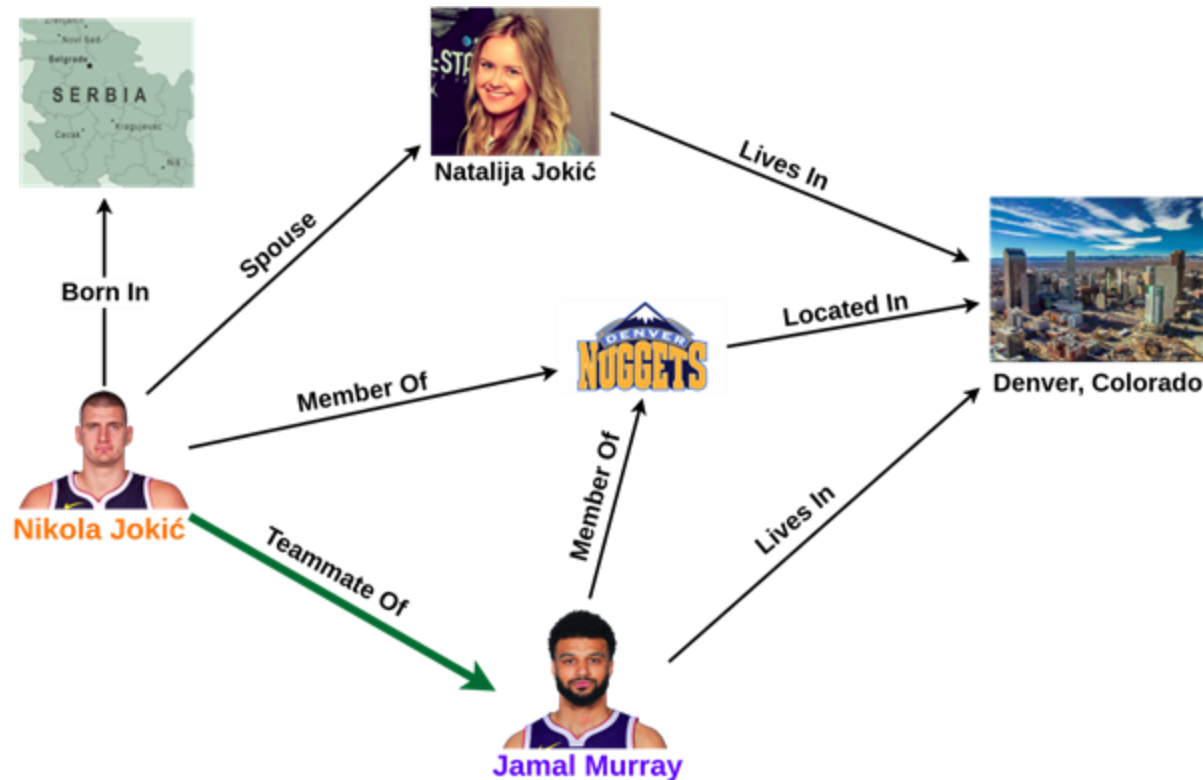
# Outline



# Knowledge Graph - What are Knowledge Graph (KGs)?

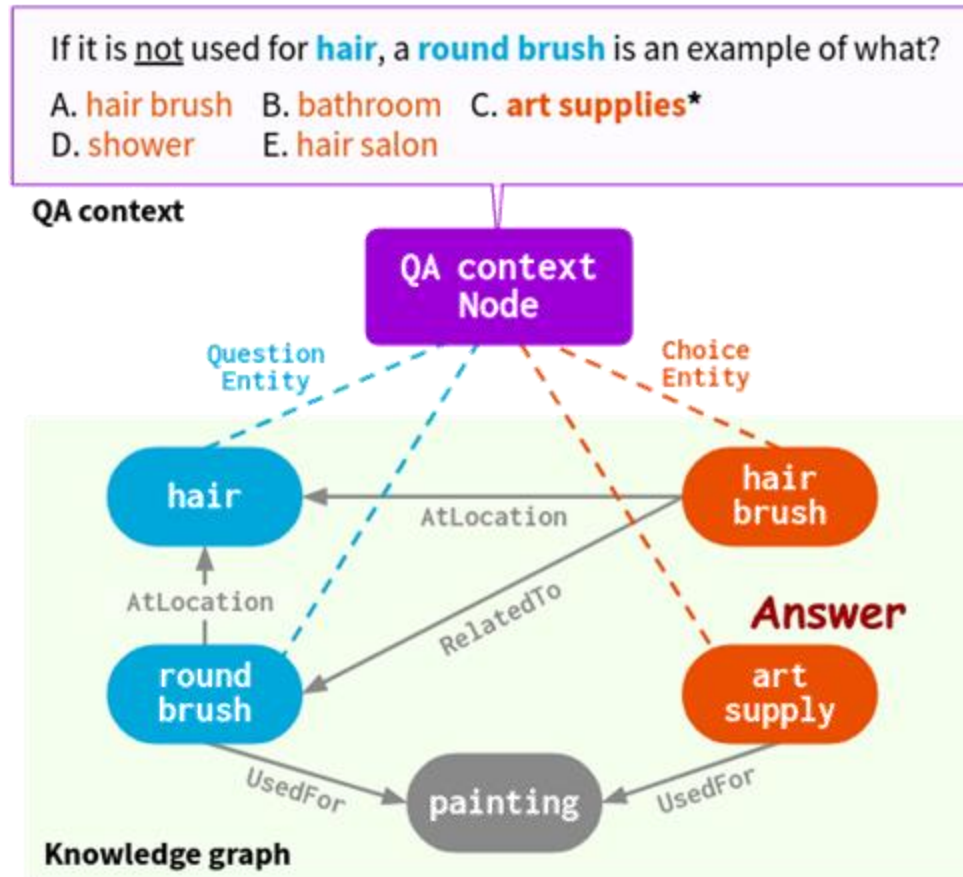


# Knowledge Graph - What are Knowledge Graph (KGs)?



# Knowledge Graph - Tasks

## Question Answering



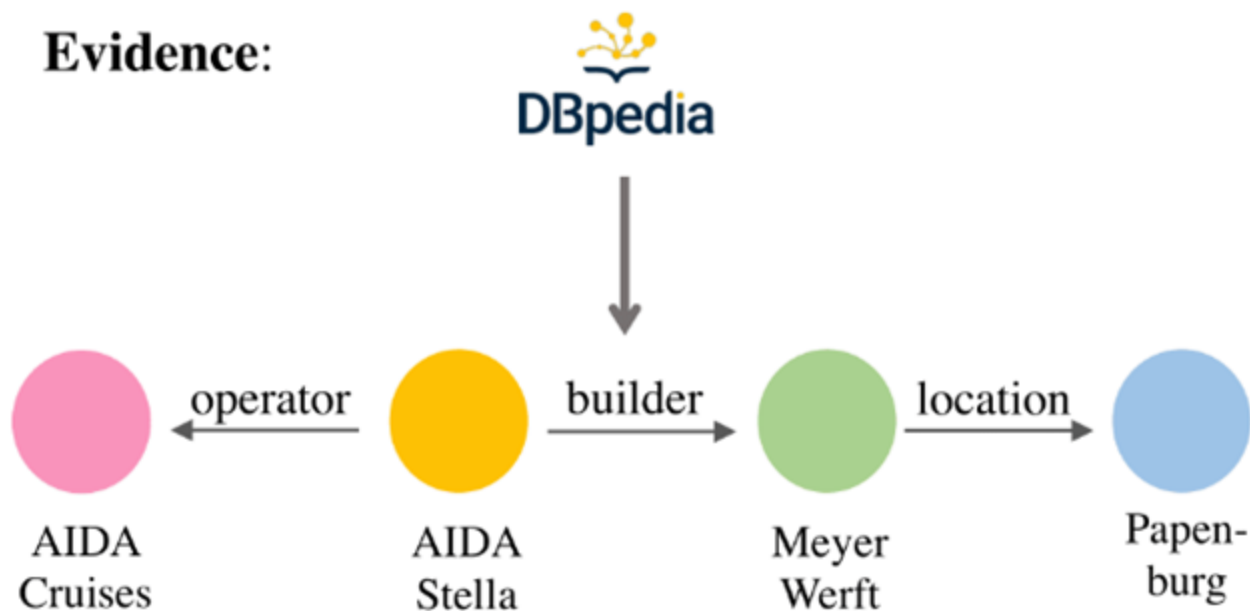
# Knowledge Graph - Tasks

## Fack Checking

**Claim:** Yeah! Actually AIDA Cruise line operated a ship which was built by a company in Papenburg!

---

**Evidence:**



---

**Label:** SUPPORTED

# Knowledge Graph - Tasks

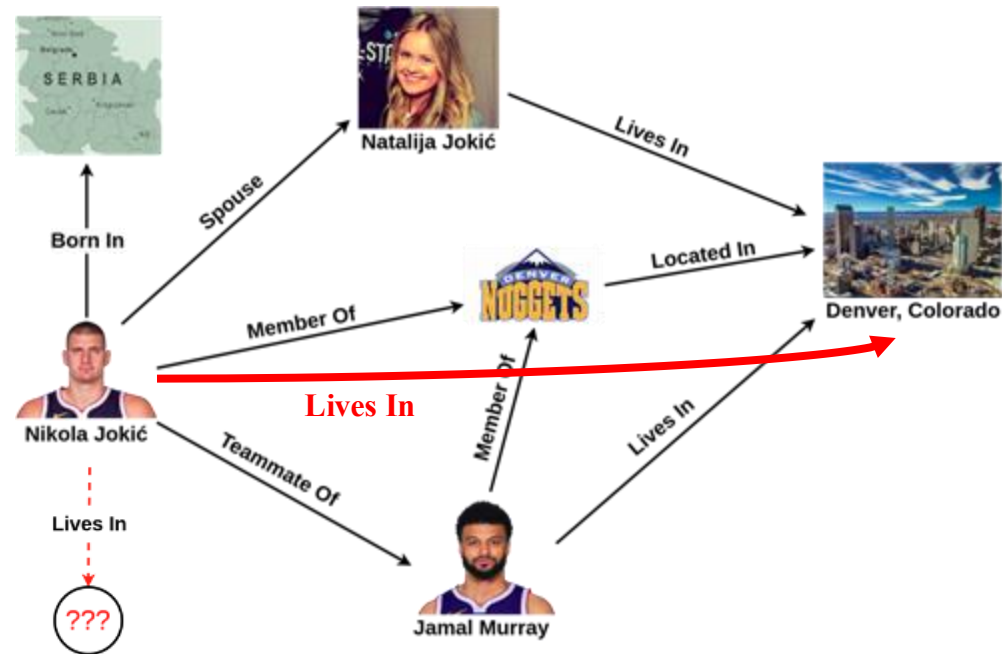
## Knowledge Graph Completion

Given:

(  , Lives In, **???** )  
Nikola Jokić

Given:

(  , Lives In,  )  
Nikola Jokić      Denver, CO



# Knowledge Graph - Using KGs for GraphRAG

Where does Nikola Jokic  
Live?

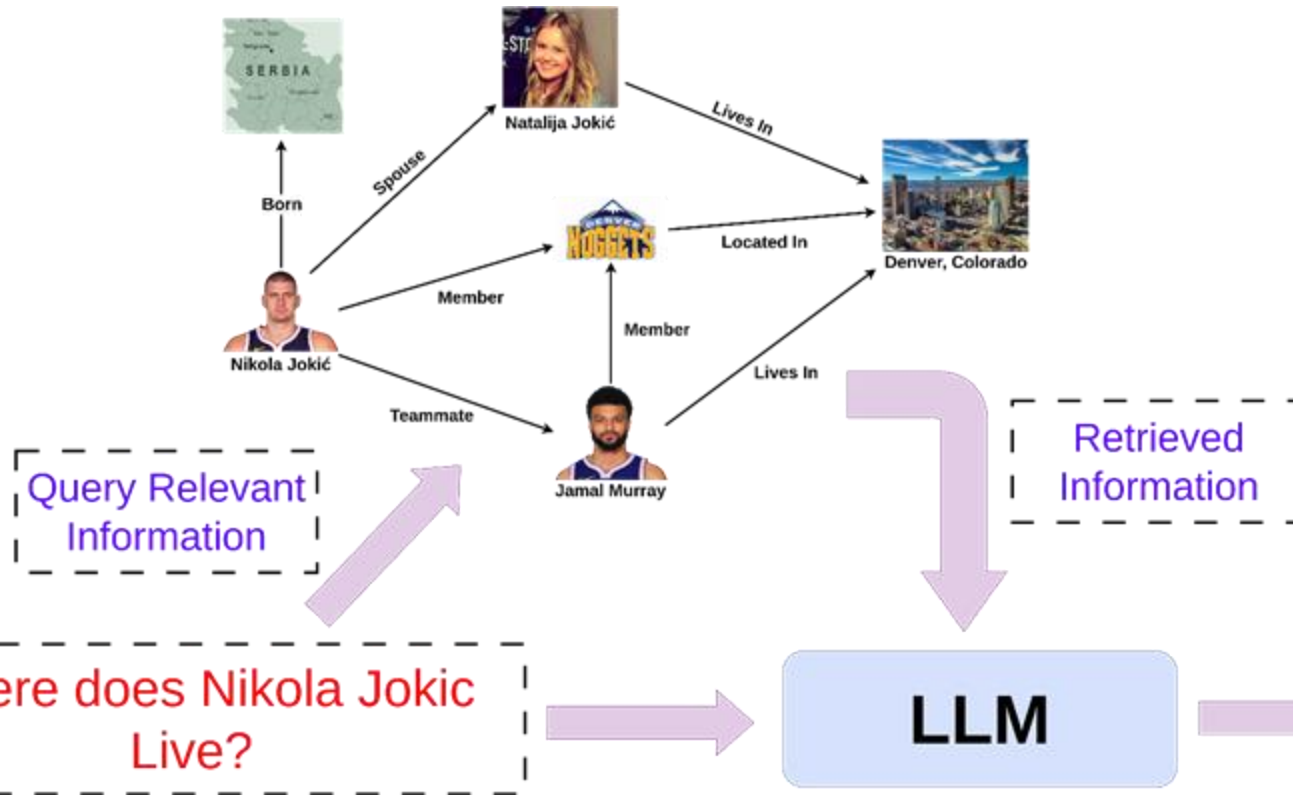


LLM



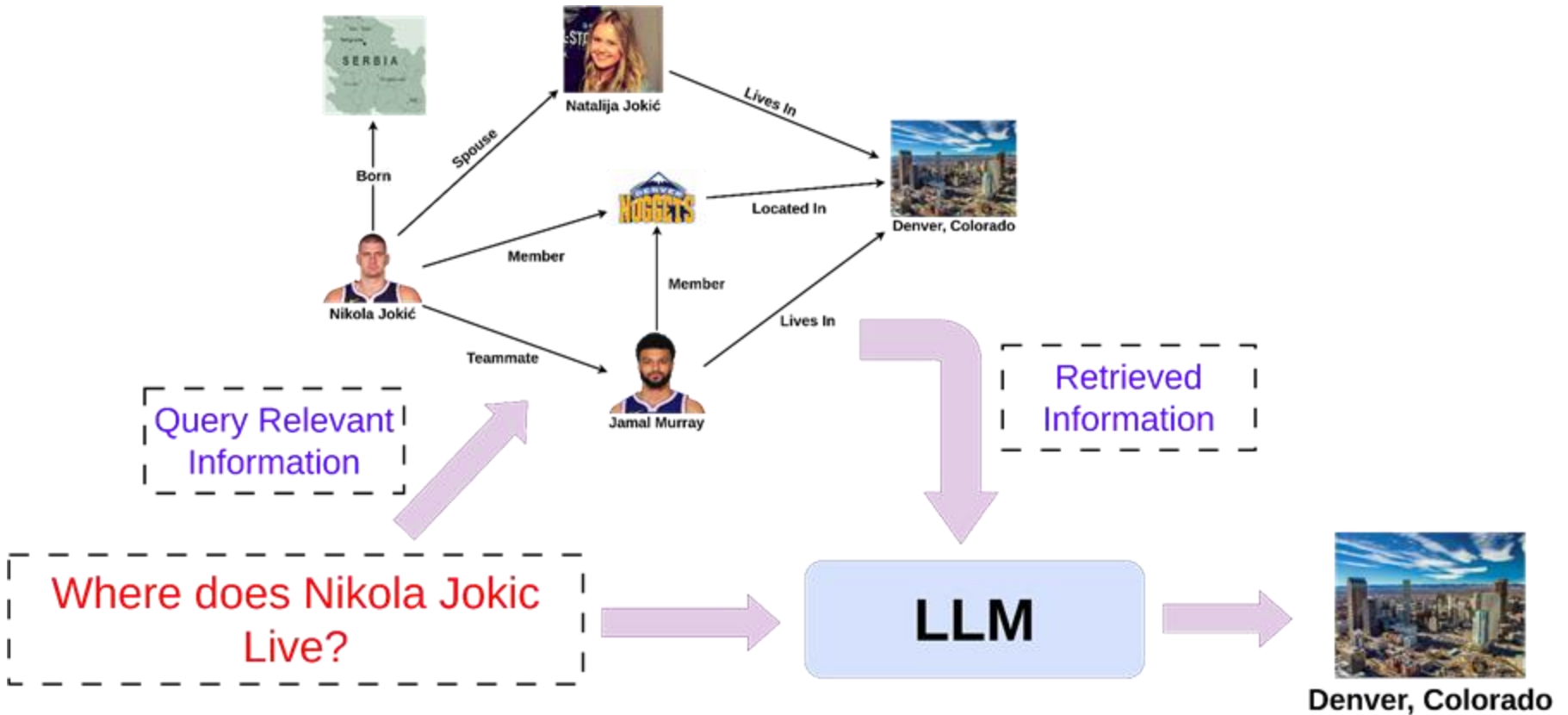
?

# Knowledge Graph - Using KGs for GraphRAG





# Knowledge Graph - Using KGs for GraphRAG



# Knowledge Graph - How are KGs are Constructed?






## 1) Manual Construction

- Done via human annotation
- Popular example is the WikiData database

# Knowledge Graph - How are KGs are Constructed?

Entity ← **Geoffrey Hinton** (Q92894)

**Facts with Hinton  
as Head Entity**

place of birth	 Wimbledon ▸ 1 reference
father	 H. E. Hinton ▸ 1 reference
languages spoken, written or signed	 English ▸ 0 references
occupation	 computer scientist ▸ 0 references
	 artificial intelligence researcher ▸ 0 references

# Knowledge Graph - How are KGs are Constructed?

## 1) Manual Construction

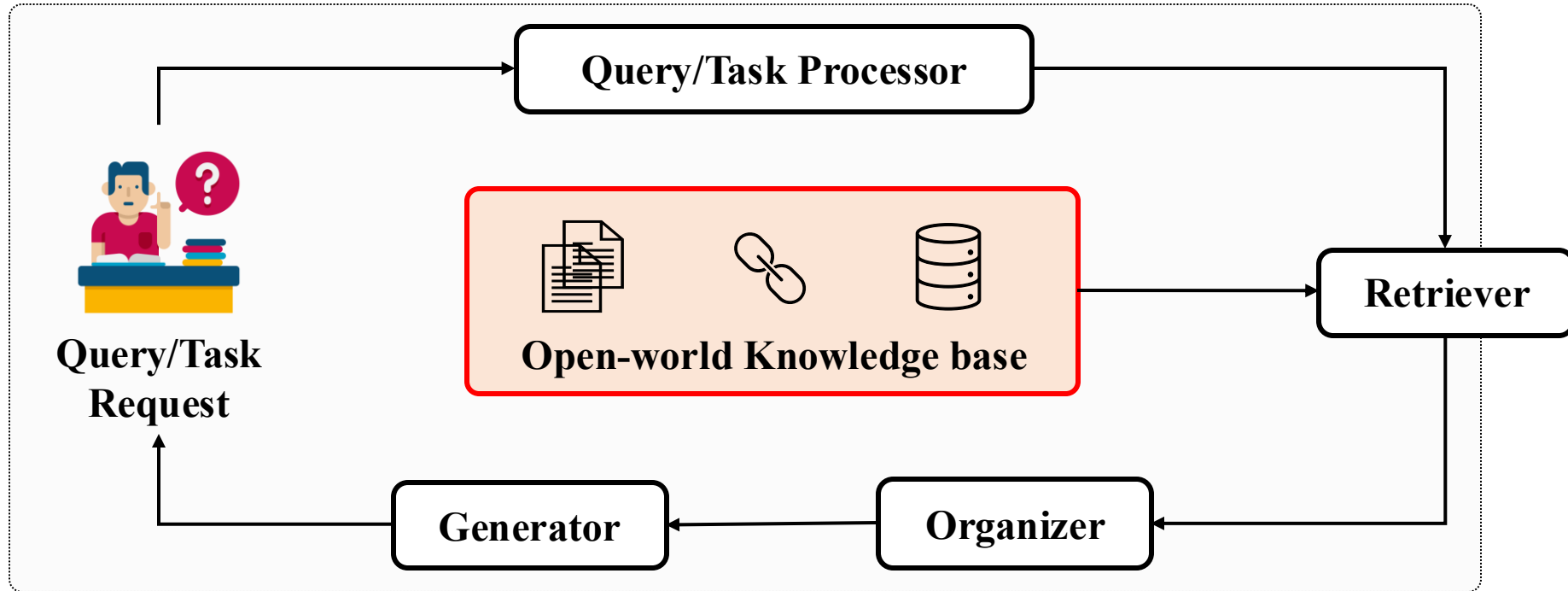
- Done via human annotation
- Popular example is the WikiData database [1]

## 2) Rule-Based Construction

## 3) LLM-Based Construction

**Covered in last section**

# Knowledge Graph - Pipeline for GraphRAG on KGs



# Knowledge Graph - GraphRAG for KGs

- A **key difference** in KG GraphRAG frameworks is the **retrieval method**
  - “*How do we retrieve relevant facts for our query?*”
- **Keys retrieval strategies:**
  - Subgraph-based
  - Traversal-based
  - GNN-based
  - Other (Agent, Semantic similarity)

# Knowledge Graph - GraphRAG for KGs

- A **key difference** in KG GraphRAG frameworks is the **retrieval method**
  - *“How do we retrieve relevant facts for our query?”*
- **Keys retrieval strategies:**
  - **Subgraph-based: MindMap [1]**
  - **Traversal-based: RoG [2]**
  - **GNN-based: SubGraphRAG [3]**
  - Other (Agent, Semantic similarity)

[1] "MindMap: Knowledge Graph Prompting Sparks Graph of Thoughts in Large Language Models". ACL 2024.

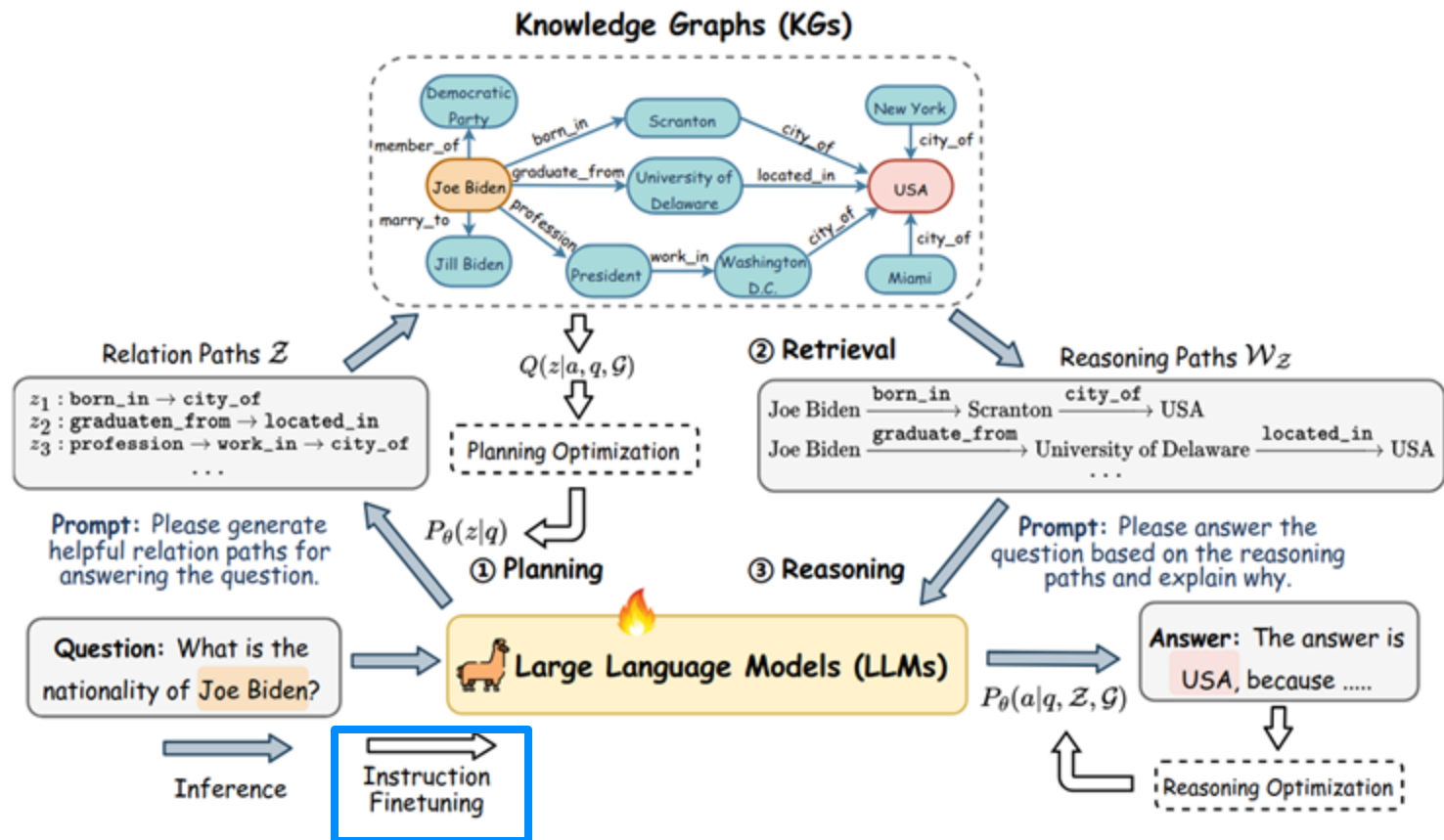
[2] "Reasoning on Graphs: Faithful and Interpretable Large Language Model Reasoning." ICLR 2024.

[3] "Simple is Effective: The Roles of Graphs and Large Language Models in Knowledge-Graph-Based Retrieval-Augmented Generation." ICLR 2025.

# Knowledge Graph - Reasoning on Graph (RoG)

**Motivation:** How to extract a subset of “faithful and reliable” paths for the query?

**Basic Idea:** Extract relevant paths from a KG for a given query

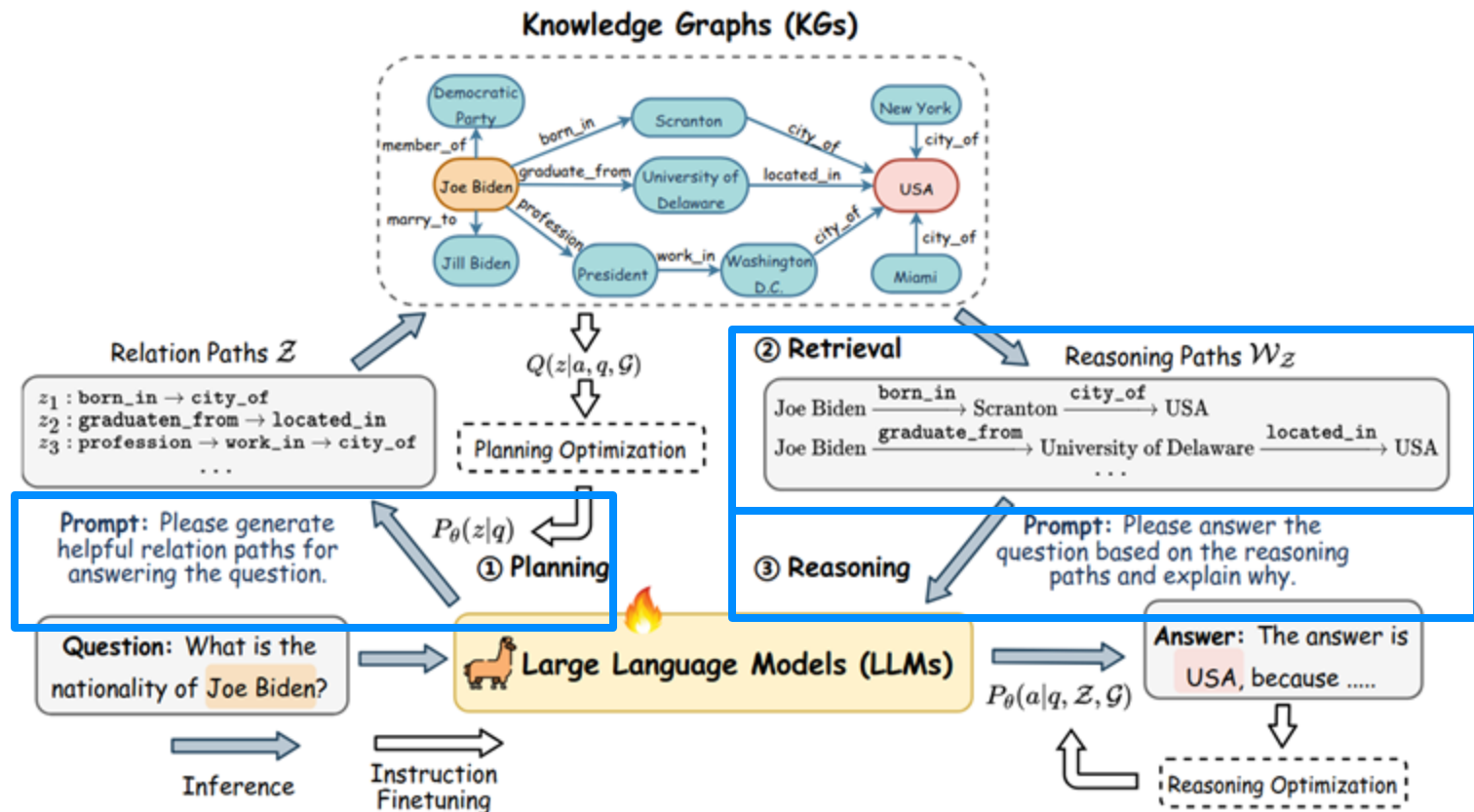




# Knowledge Graph - Reasoning on Graph (RoG)

**Motivation:** How to extract a subset of “faithful and reliable” paths for the query?

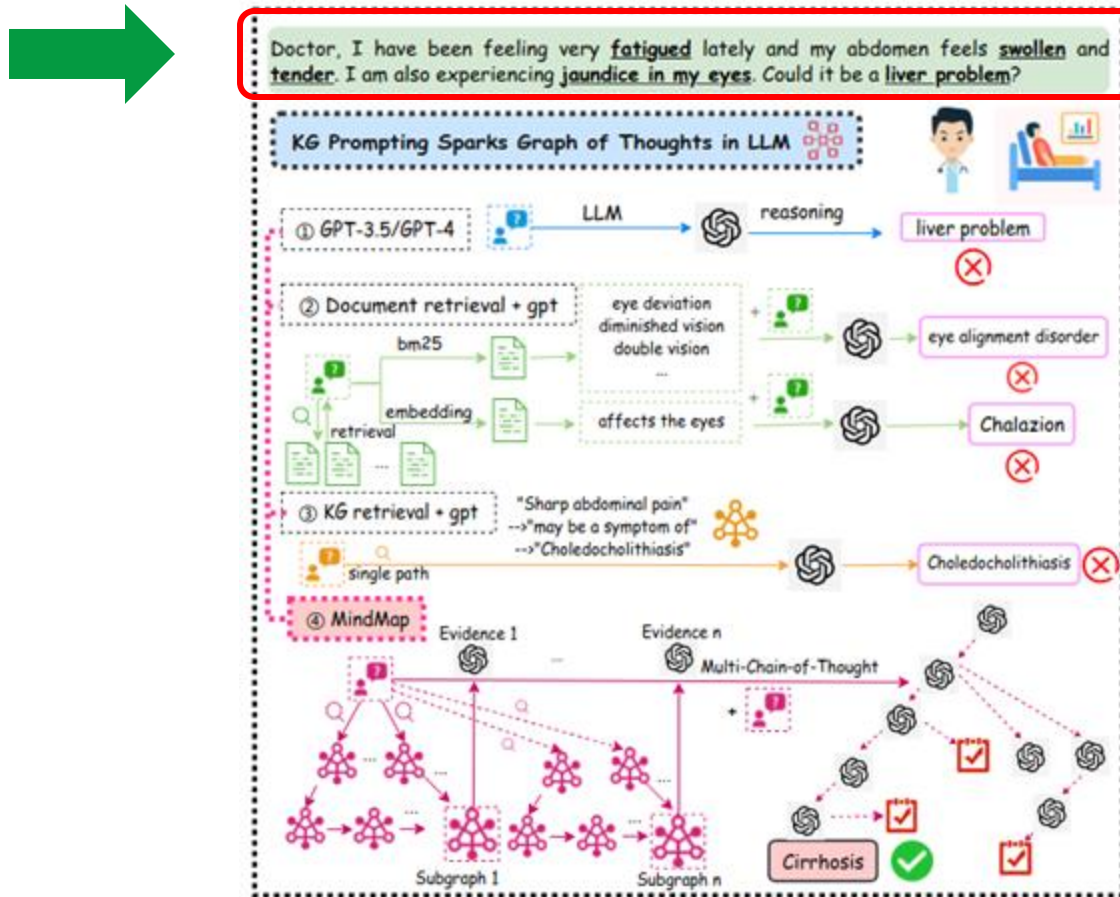
**Basic Idea:** Extract paths that follow specific templates, outputted by a LLM



# Knowledge Graph - MindMap

**Motivation:** Explainable and diverse reasoning process to mitigate hallucinations

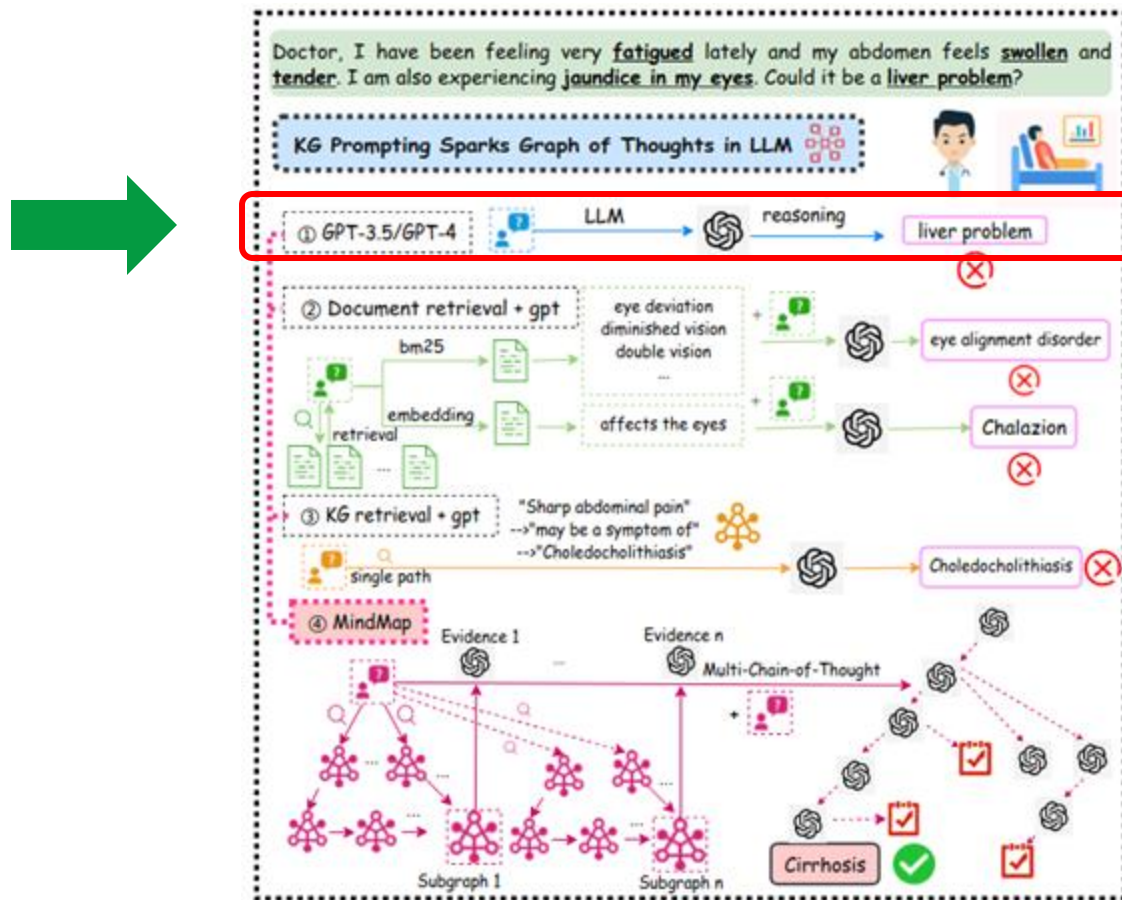
**Basic Idea:** For a query, extract both relevant subgraphs and paths



# Knowledge Graph - MindMap

**Motivation:** Explainable and diverse reasoning process to mitigate hallucinations

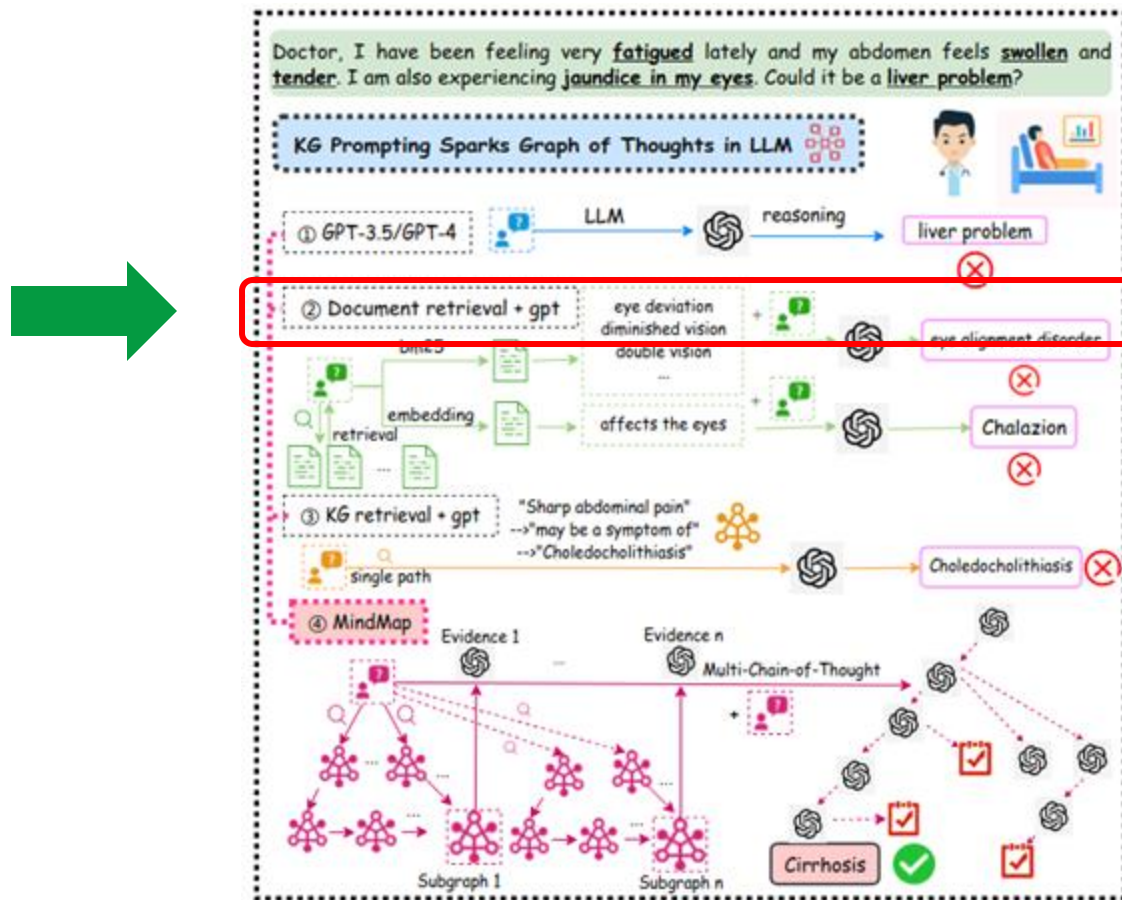
**Basic Idea:** For a query, extract both relevant subgraphs and paths



# Knowledge Graph - MindMap

**Motivation:** Explainable and diverse reasoning process to mitigate hallucinations

**Basic Idea:** For a query, extract both relevant subgraphs and paths



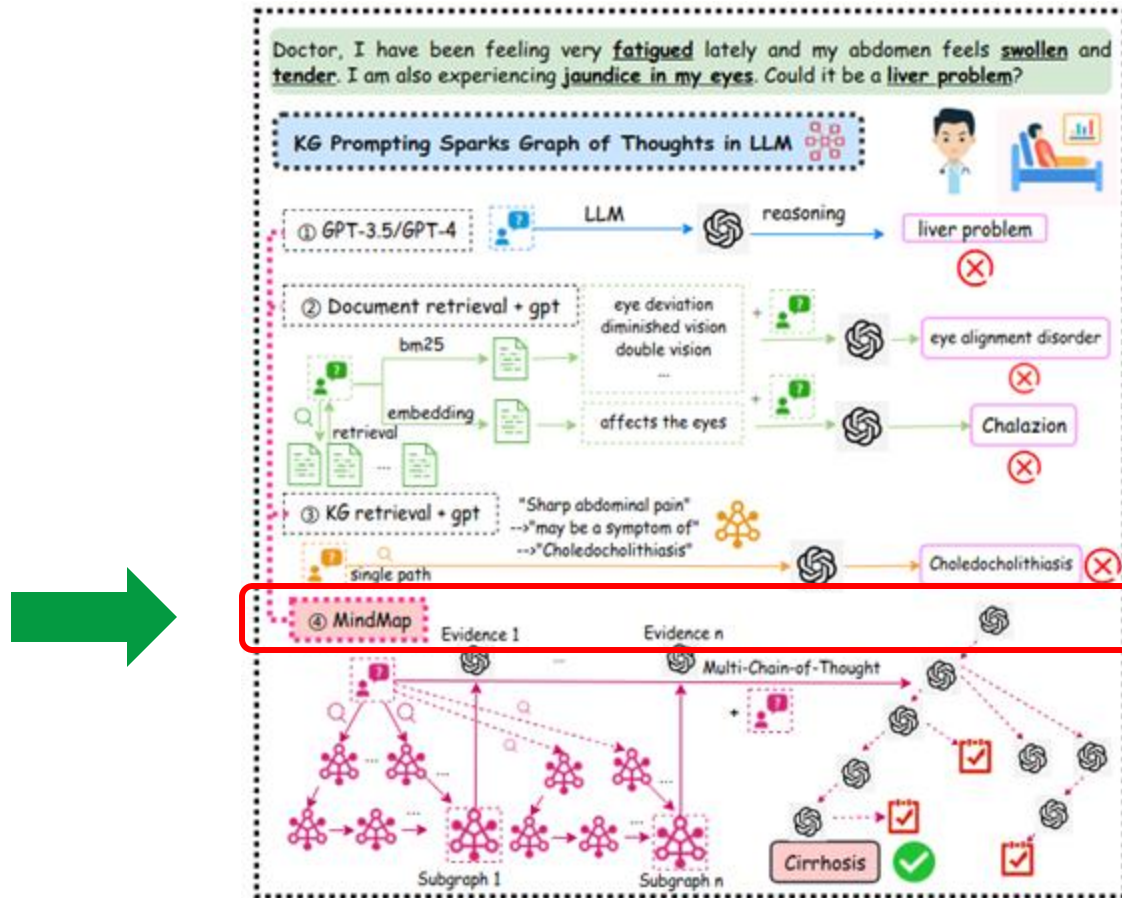




# Knowledge Graph - MindMap

**Motivation:** Explainable and diverse reasoning process to mitigate hallucinations

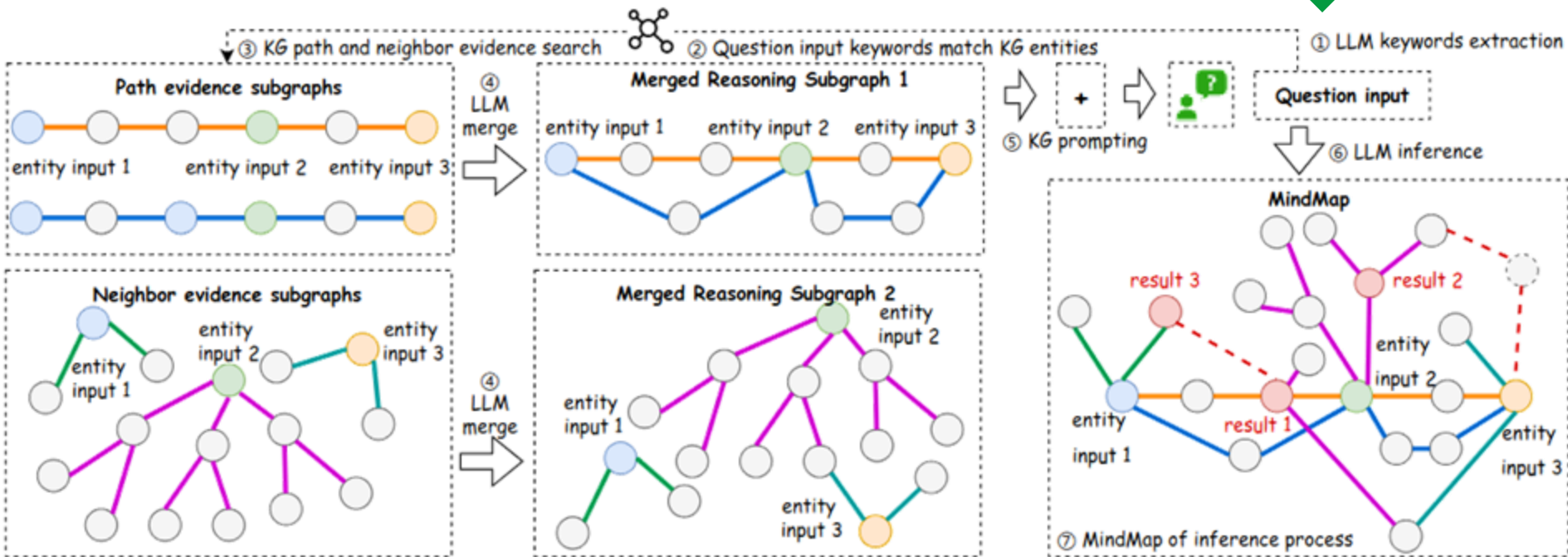
**Basic Idea:** For a query, extract both relevant subgraphs and paths



# Knowledge Graph - MindMap

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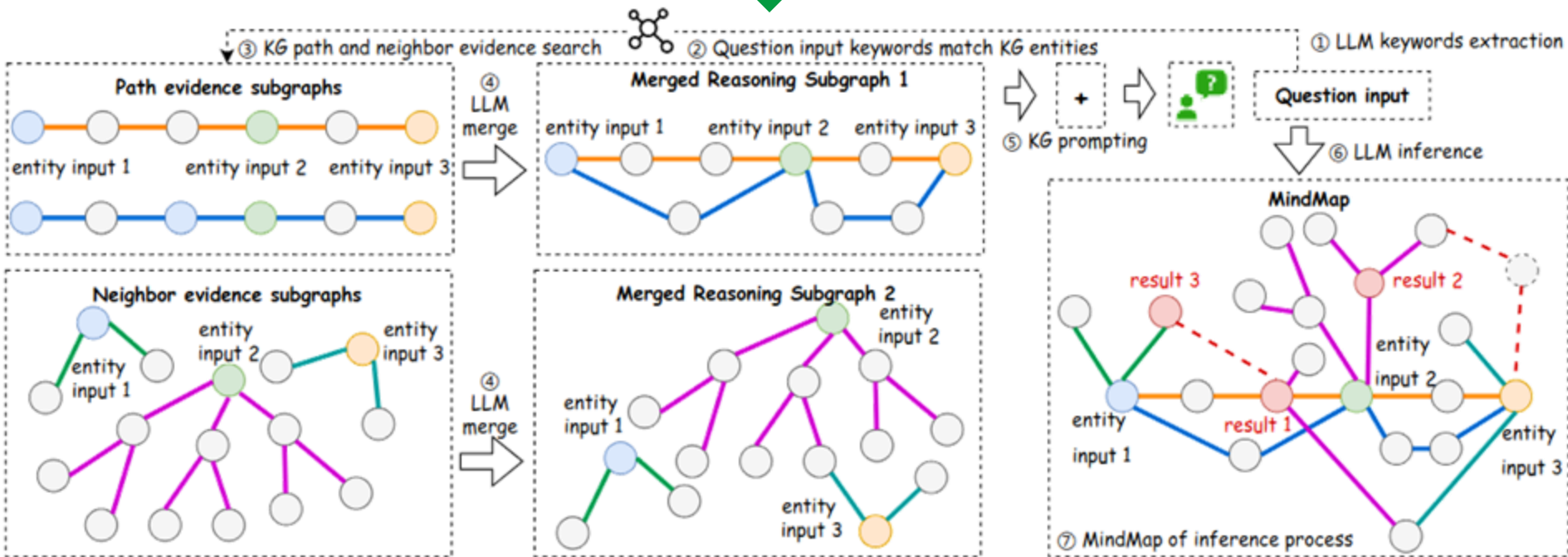
**Basic Idea:** For a query, extract both relevant subgraphs and paths



# Knowledge Graph - MindMap

**Motivation:** Explainable and diverse reasoning process to mitigate hallucinations

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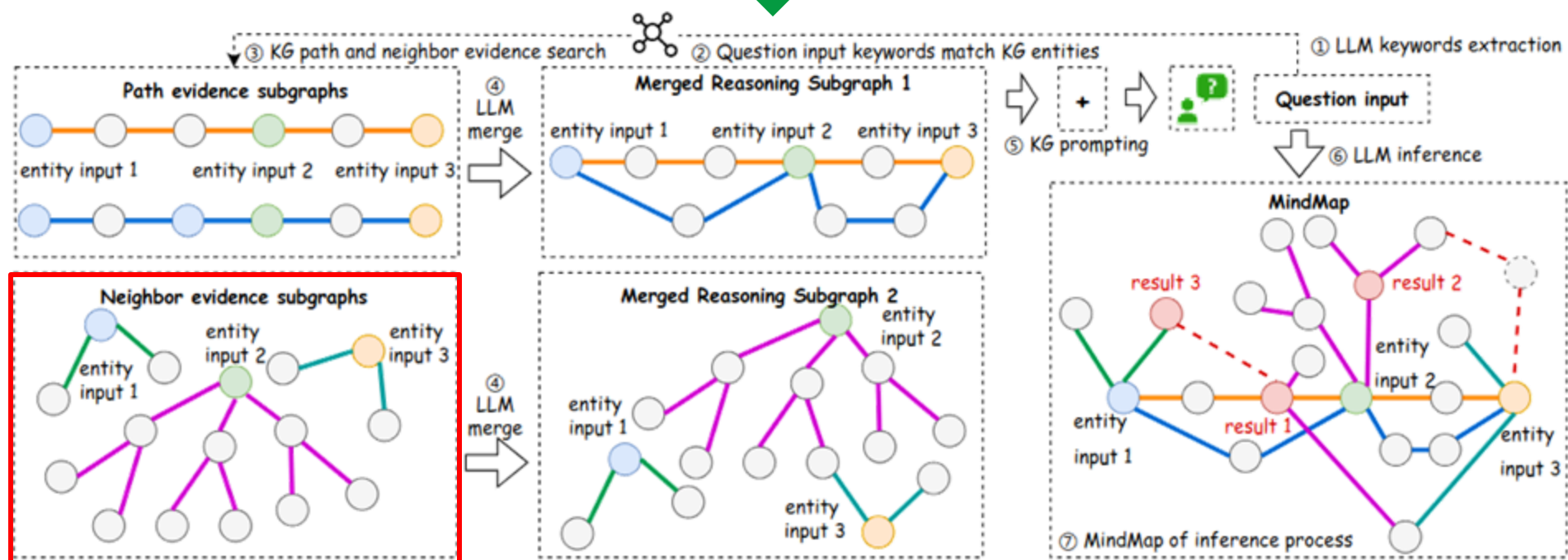




# Knowledge Graph - MindMap

**Motivation:** Explainable and diverse reasoning process to mitigate hallucinations

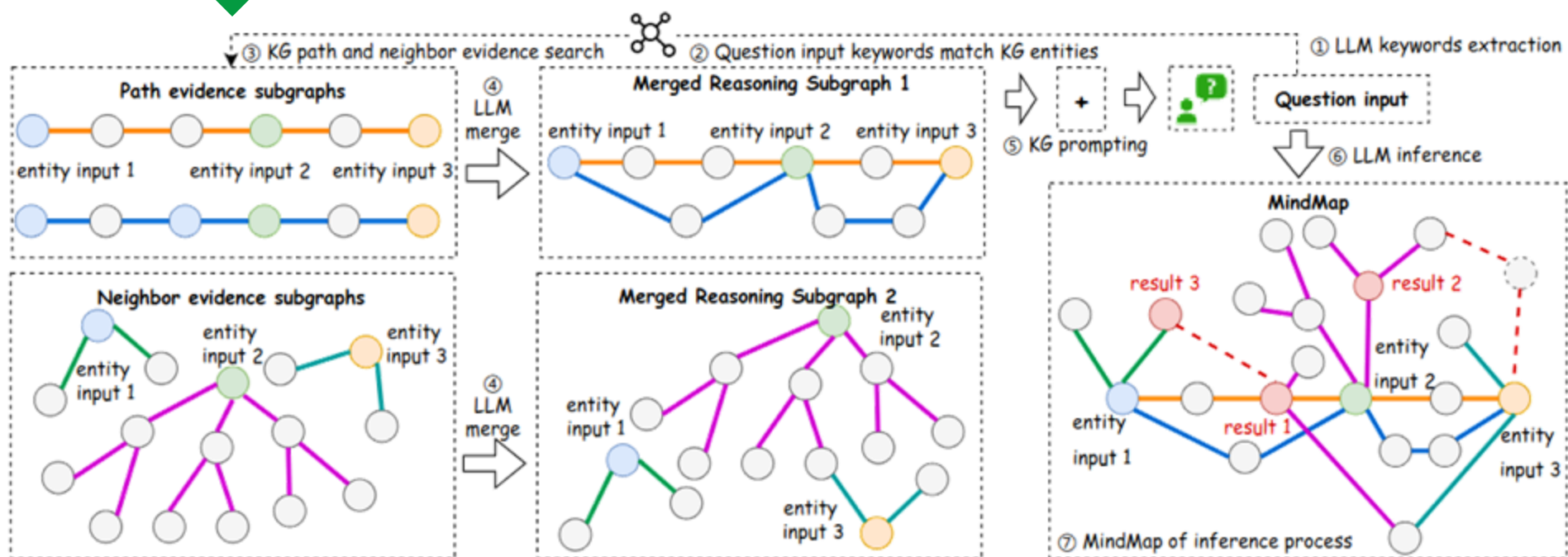
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# Knowledge Graph - MindMap

**Motivation:** Explainable and diverse reasoning process to mitigate hallucinations

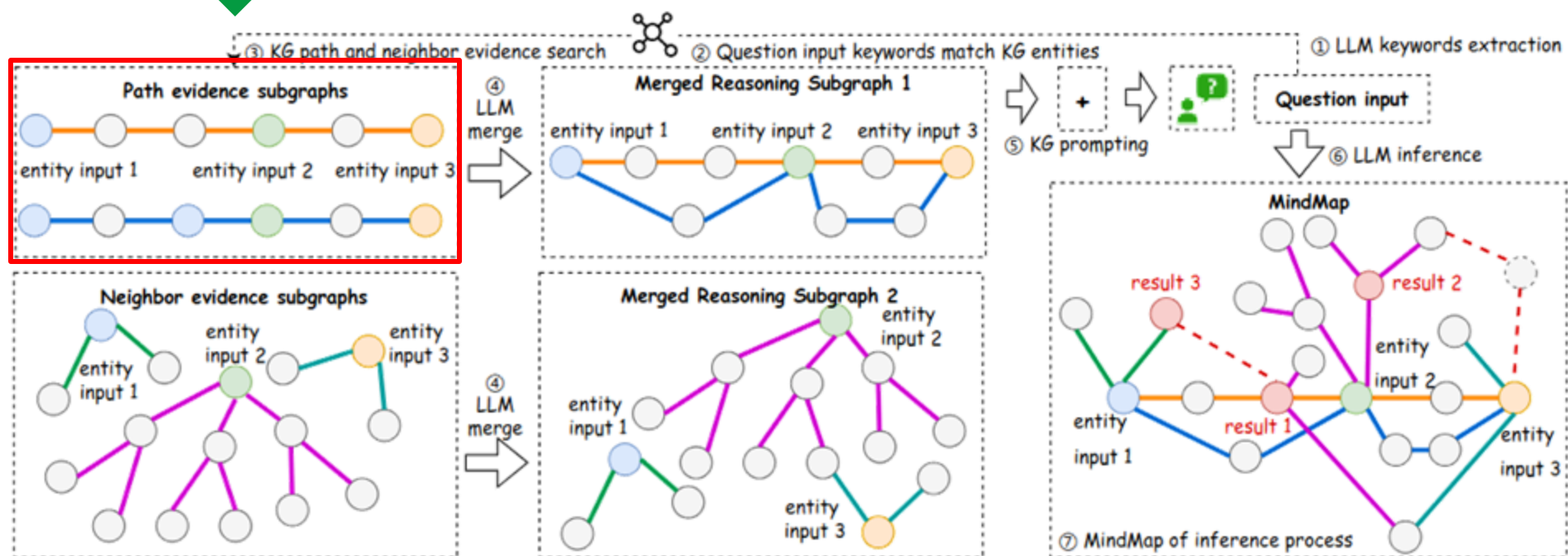
**Basic Idea:** For a query, extract both relevant subgraphs and paths



# Knowledge Graph - MindMap

**Motivation:** Explainable and diverse reasoning process to mitigate hallucinations

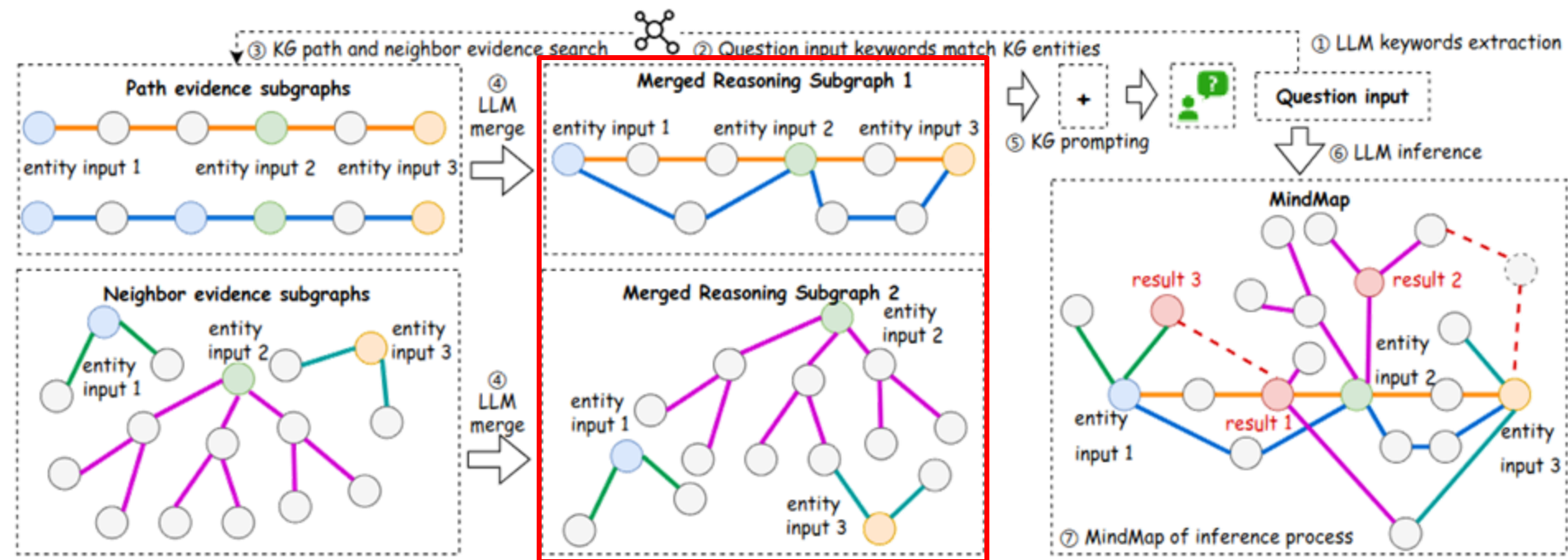
**Basic Idea:** For a query, extract both relevant subgraphs and paths



# Knowledge Graph - MindMap

**Motivation:** Explainable and diverse reasoning process to mitigate hallucinations

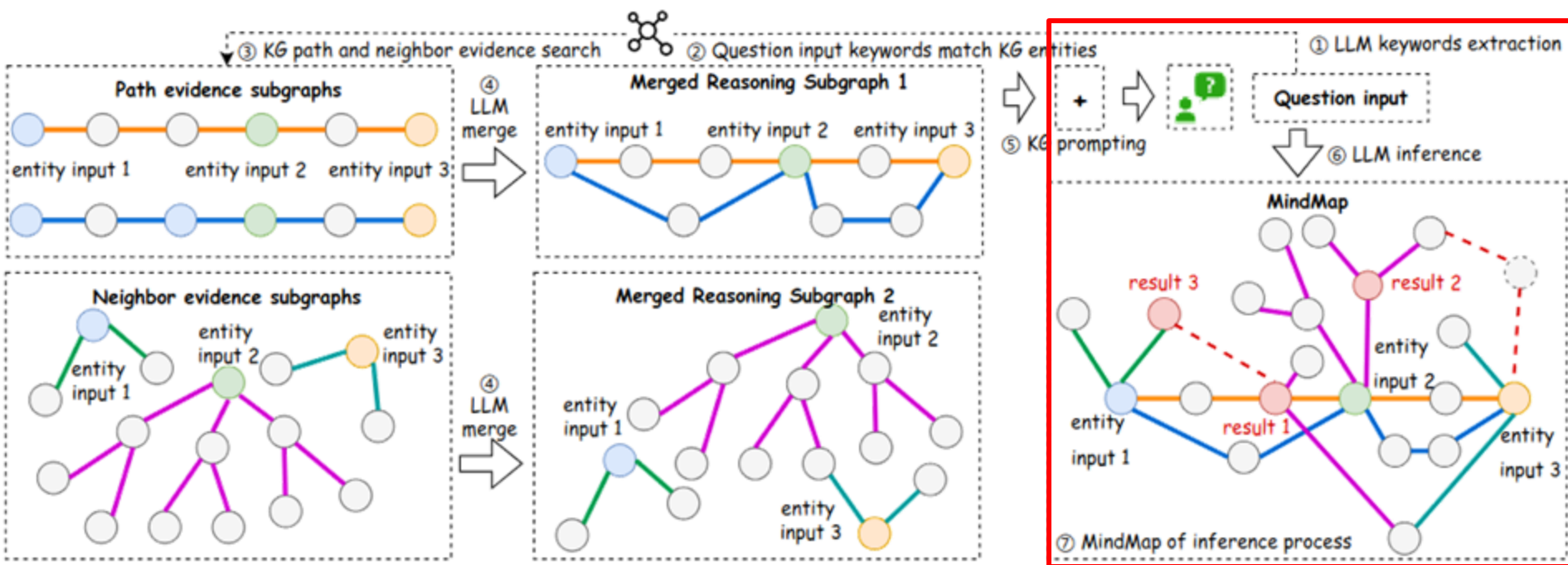
**Basic Idea:** For a query, extract both relevant subgraphs and paths



# Knowledge Graph - MindMap

**Motivation:** Explainable and diverse reasoning process to mitigate hallucinations

**Basic Idea:** For a query, extract both relevant subgraphs and paths



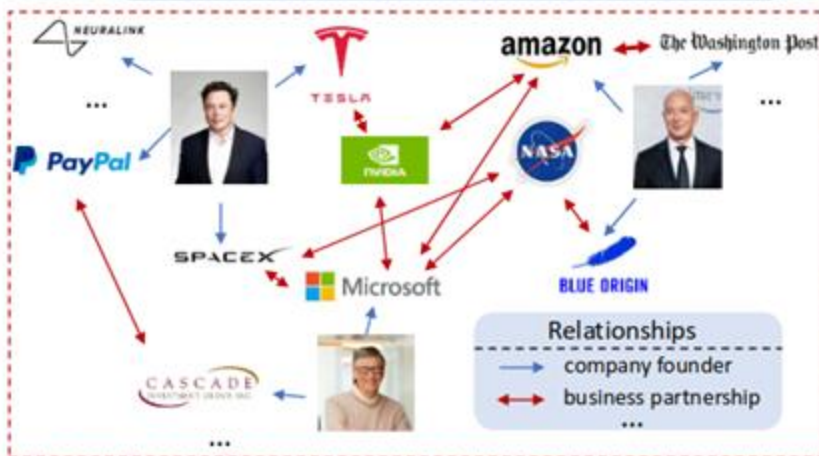


# Knowledge Graph - SubGraphRAG

**Motivation:** There is a tradeoff between retrieval efficiency and reasoning abilities

**Basic Idea:** Use a GNN to learn how to extract the important paths for the query

“Which organizations have business partnerships with at least one company founded respectively by **Elon Musk**, **Jeff Bezos**, and **Bill Gates** - but weren't founded by any of them?”



## SubgraphRAG

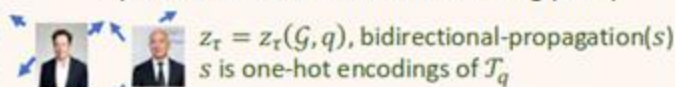
**Step 1 - Topic entity  $\mathcal{T}_q$  extraction:**



**Step 2 - Subgraph  $\mathcal{G}_q$  extraction:**

**Step 2.1 - Structural Feature Construction**

Option 1: Directional Distance Encoding (used)



Option 2: GNNs (not used)

**Step 2.2 - Extract Relevant Triples in Parallel**

Top  $K$  triples in  $\{ \left( \text{Elon Musk} \rightarrow \text{Tesla} \right) \left( \text{Tesla} \leftrightarrow \text{NVIDIA} \right) \dots \}$   
 $p_\theta(\tau|z_\tau, q)$

**Step 3 - LLMs for reasoning over  $\mathcal{G}_q$ :**

“Use the triples in the list as evidence to answer the question”



The list of answers:  
**[Nvidia, Nasa]**

The reasoning is as follows.

**Nvidia** has **business partnerships** with:

1. Tesla **founded by** Elon Musk
2. Amazon **founded by** Jeff Bezos
3. Microsoft **founded by** Bill Gates

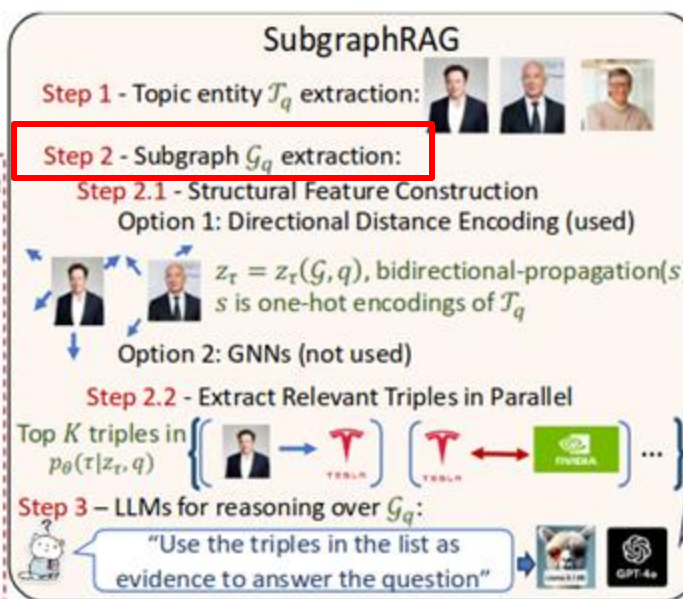
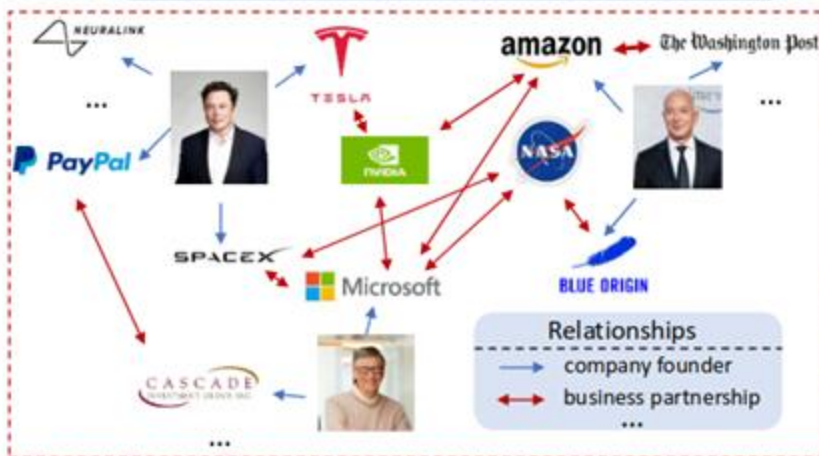
**Nvidia** was not founded by Elon Musk, Jeff Bezos, or Bill Gates.

# Knowledge Graph - SubGraphRAG

**Motivation:** There is a tradeoff between retrieval efficiency and reasoning abilities

**Basic Idea:** Use a GNN to learn how to extract the important paths for the query

“Which organizations have business partnerships with at least one company founded respectively by **Elon Musk**, **Jeff Bezos**, and **Bill Gates** - but weren't founded by any of them?”



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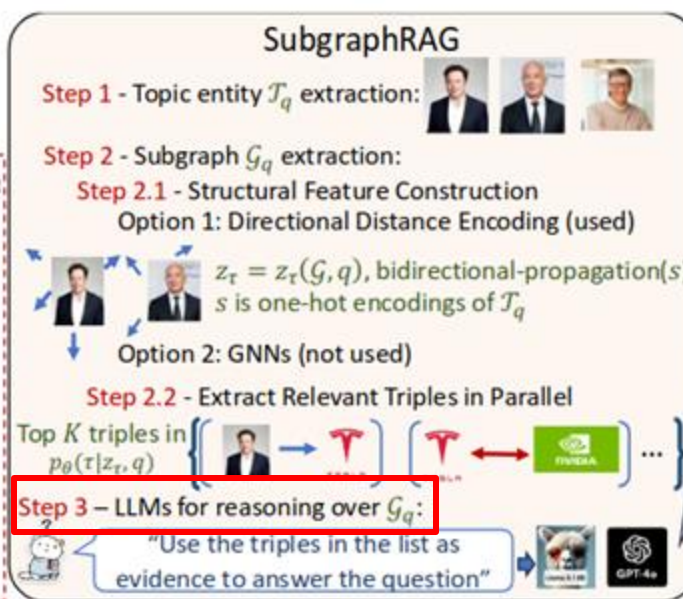
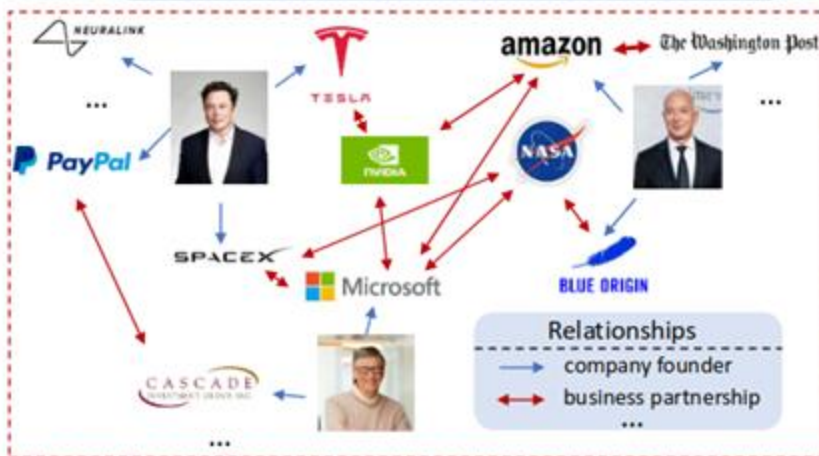
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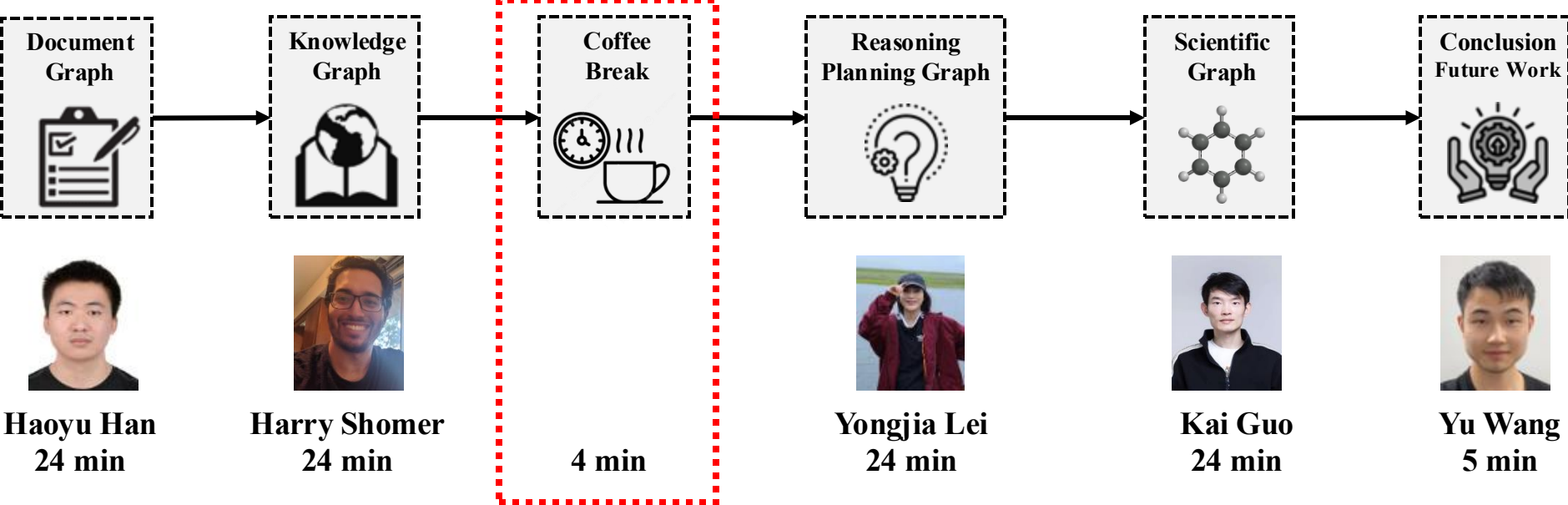
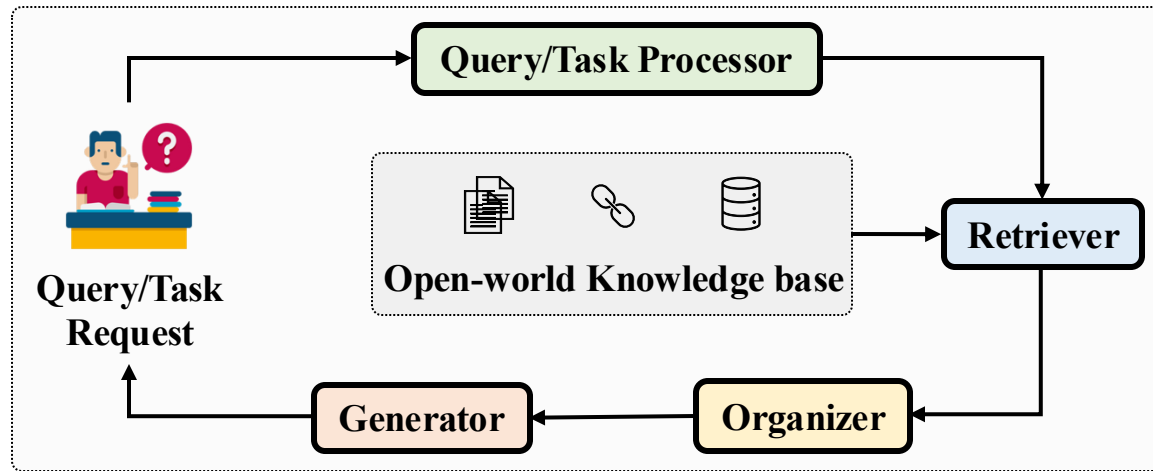


# Knowledge Graph - Future Work

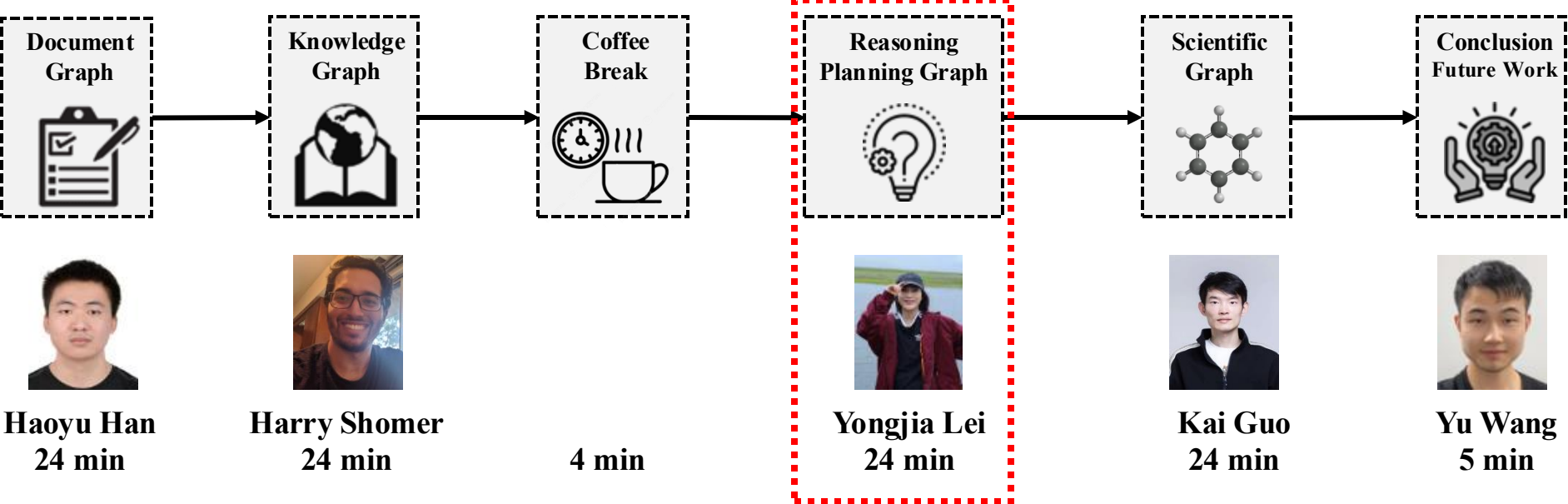
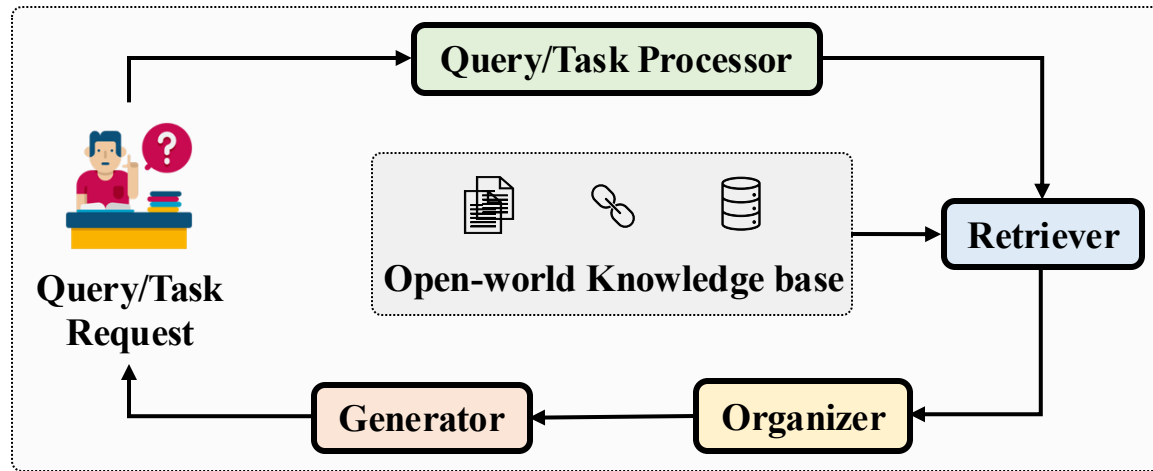
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1. How to best **construct** KGs? What granularity should the node/edges be?
2. How do we **harmonize** the internal LLM knowledge and retrieved KG knowledge?
3. What's the best way of **organizing** the triples or paths for the LLM?

# Outline



# Outline



# Reasoning & Planning Graph

## What is Reasoning?

Thinking logically and systematically

Using Evidence/past experiences for drawing conclusion and decision-making

## What is Planning?

Formulating a series of actions or operations to achieve a specific goal.

**Reasoning and Planning are deeply interconnected in RAG**

### Make Calzones

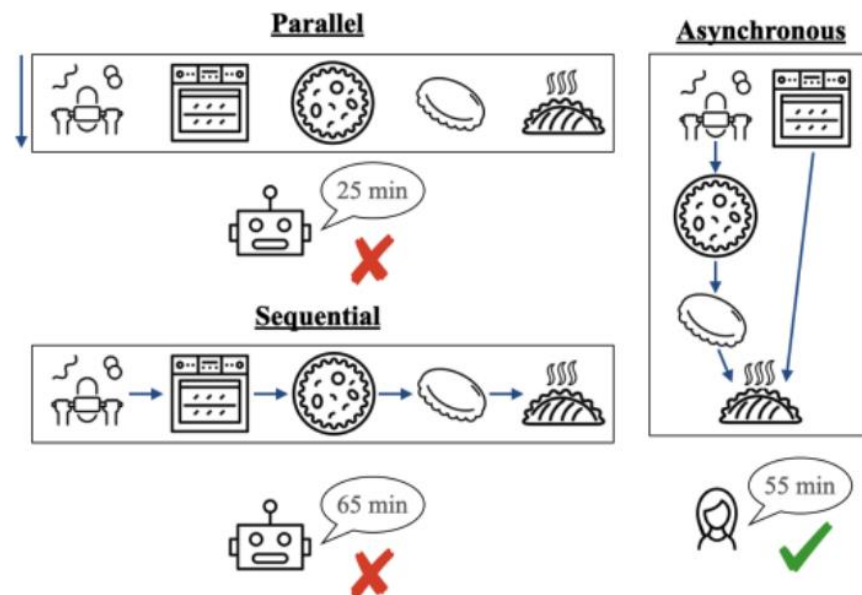
Preheat the oven to 425 degrees – **10 minutes**

Roll out the dough – **10 minutes**

Add the filling – **15 minutes**

Fold and pinch the dough – **5 minutes**

Bake the calzones – **25 minutes**

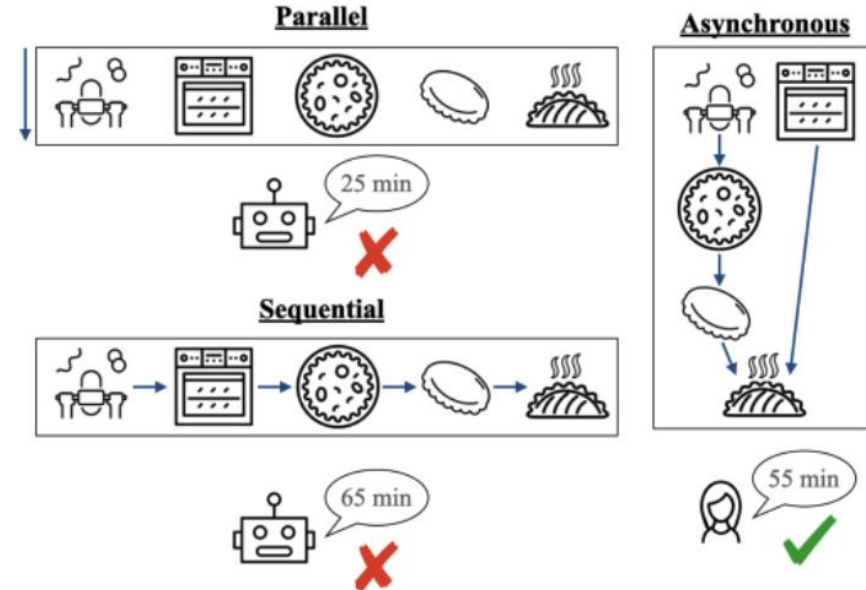
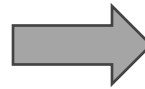


# Reasoning & Planning Graph

## Reasoning and Planning are deeply interconnected in RAG

### Make Calzones

Preheat the oven to 425 degrees – **10 minutes**  
Roll out the dough – **10 minutes**  
Add the filling – **15 minutes**  
Fold and pinch the dough – **5 minutes**  
Bake the calzones – **25 minutes**



- Retrieving task components, e.g., actions, time
- Reasoning about dependencies
- Planning the execution order

# Reasoning & Planning Graph

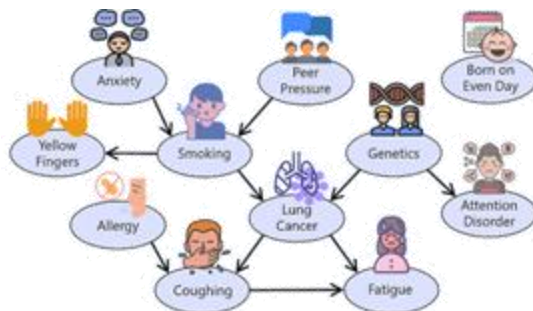
## Why Reasoning and Planning Graphs are Important in GraphRAG?

- Dependences/sequences to capture relations, e.g., Causal and Resource Dependency
- Structuring the Retrieval Process



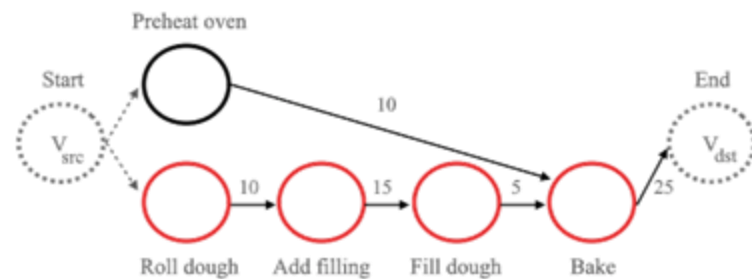
**Resource Dependency**

[Shen et al. 2024](#)



**Causal Dependency**

[LUCAS 2024](#)



**Temporal Dependency**

[Lin 2024](#)

## Common Dependencies in Graph Construction

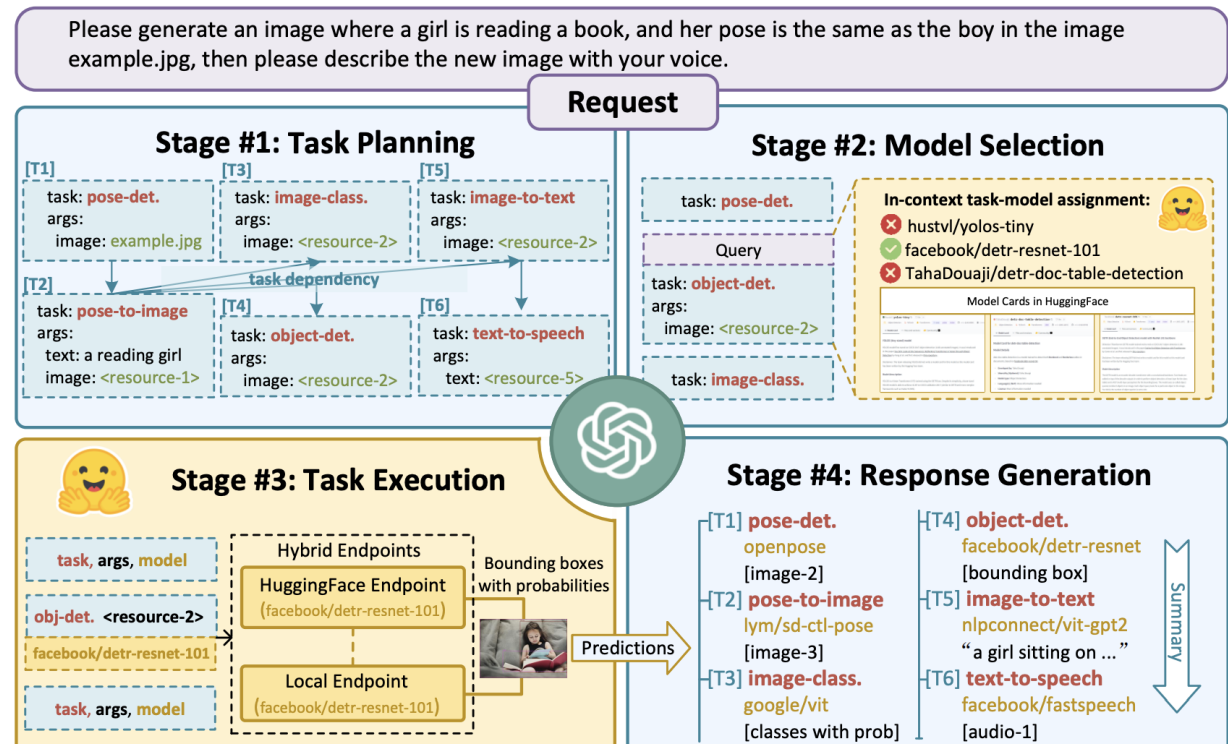
# Reasoning & Planning Graph – Task Planning

**Task Planning:** Retrieve/generate plan of steps/tools in graph format

## Planning Graph:

- Capture dependencies and execution orders
- Guide APIs retrieval
- Guide inter-model cooperation

## HuggingGPT: Generation-based Planning



# Reasoning & Planning Graph – Task Planning

## How to enable LLMs conduct task planning?

- Specification-based Instruction
- Demonstration-based Parsing

Prompt	
<p>#1 Task Planning Stage - The AI assistant performs task parsing on user input, generating a list of tasks with the following format: <code>{"task": task, "id": task_id, "dep": dependency_task_ids, "args": {"text": text, "image": URL, "audio": URL, "video": URL}}</code>. The "dep" field denotes the id of the previous task which generates a new resource upon which the current task relies. The tag <code>&lt;resource&gt;-task_id</code> represents the generated text, image, audio, or video from the dependency task with the corresponding task_id. The task must be selected from the following options: <code>{{ Available Task List }}</code>. Please note that there exists a logical connections and order between the tasks. In case the user input cannot be parsed, an empty JSON response should be provided. Here are several cases for your reference: <code>{{ Demonstrations }}</code>. To assist with task planning, the chat history is available as <code>{{ Chat Logs }}</code>, where you can trace the user-mentioned resources and incorporate them into the task planning stage.</p>	
Demonstrations	
Can you tell me how many objects in e1.jpg?	<code>[{"task": "object-detection", "id": 0, "dep": [-1], "args": {"image": "e1.jpg" }}]</code>
In e2.jpg, what's the animal and what's it doing?	<code>[{"task": "image-to-text", "id": 0, "dep": [-1], "args": {"image": "e2.jpg" }}, {"task": "image-cls", "id": 1, "dep": [-1], "args": {"image": "e2.jpg" }}, {"task": "object-detection", "id": 2, "dep": [-1], "args": {"image": "e2.jpg" }}, {"task": "visual-question-answering", "id": 3, "dep": [-1], "args": {"text": "what's the animal doing?", "image": "e2.jpg" }}]</code>
First generate a HED image of e3.jpg, then based on the HED image and a text "a girl reading a book", create a new image as a response.	<code>[{"task": "pose-detection", "id": 0, "dep": [-1], "args": {"image": "e3.jpg" }}, {"task": "pose-text-to-image", "id": 1, "dep": [0], "args": {"text": "a girl reading a book", "image": "&lt;resource&gt;-0" }}]</code>



# Reasoning & Planning Graph – Task Planning

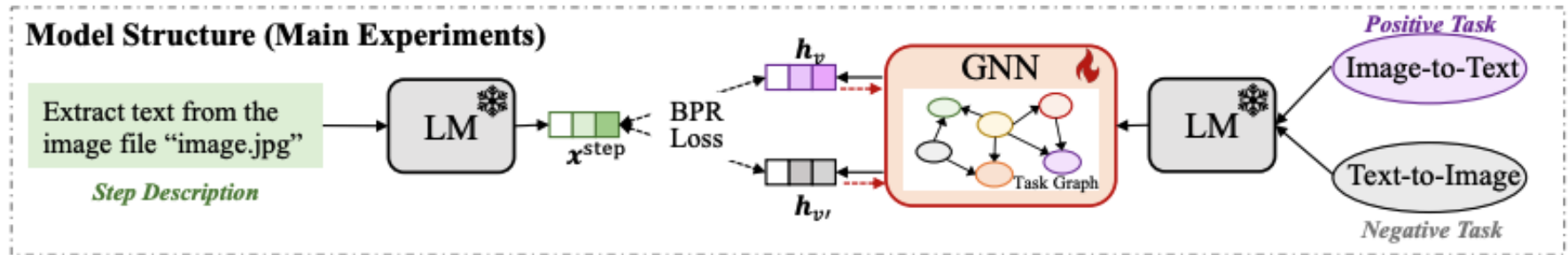
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## Challenges of Generation-based Task Planning

- Hallucinate non-existent tasks or dependencies (edges)
- Not invariant to graph isomorphism
- Performance degrades as the task graph scales

# Reasoning & Planning Graph – Task Planning

## Retrieval-based Task Planning



- Small frozen LM embeds sub-steps/task nodes in the pre-built task graph
- A GNN is applied over the task graph
  - Propagate information via pre-built dependencies
  - Refine node embeddings
- Retrieve matching tasks in the pre-built graph for sub-steps via similarity

# Reasoning & Planning Graph – Multi-Step Reasoning

**Multi-step Reasoning:** Solving problems via multiple calculations/steps

**Question:** Which publications from Altair Engineering authors focus on improving directional sensitivity across a wide range of frequencies?



**Institution** < *Altair Engineering* > → **Author** → **Paper** < *improving directional sensitivity across a wide range of frequencies* >



**Institution**



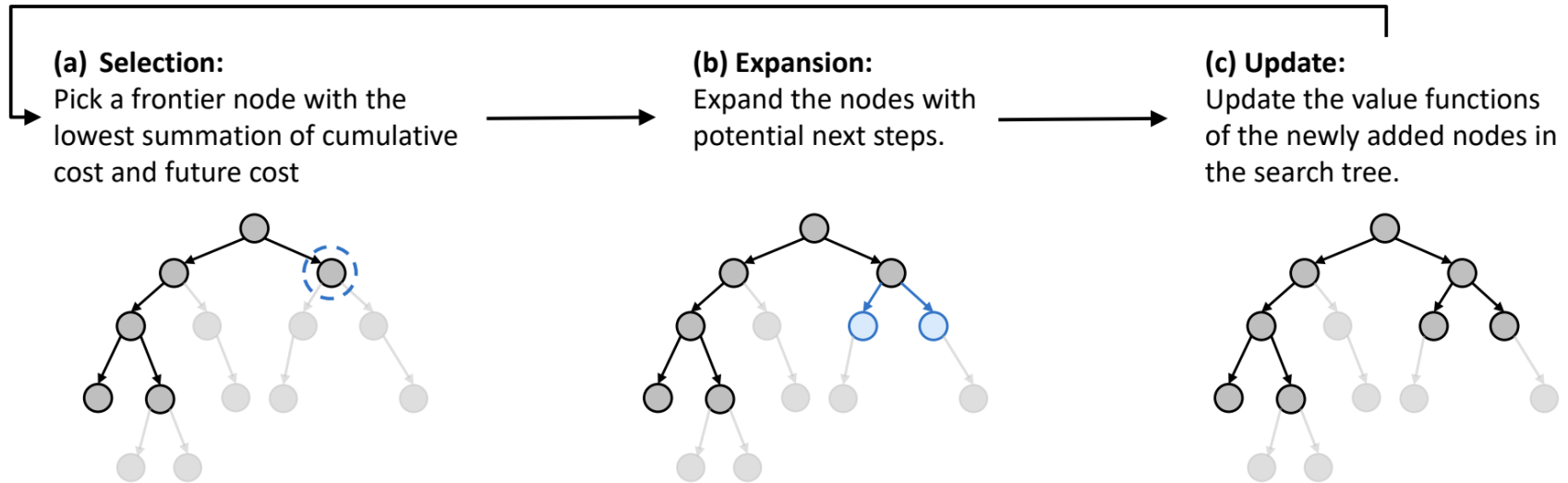
**Author**



**Paper**

# Reasoning & Planning Graph – Multi-Step Reasoning

## Toolchain\*: Efficient Action Space Navigation



**Multi-step Reasoning → Graph Search; Node → API Function Call; Edge → Possible Transition**

### Monte Carlo Tree Search vs. A\* Search

- A\*: one-step based on cost function
$$f(n) = g(n) + h(n)$$
  - $g(n)$  cumulative cost from the root node to the current node  $n$
  - $h(n)$  heuristic estimation of the future cost from node  $n$  to the goal

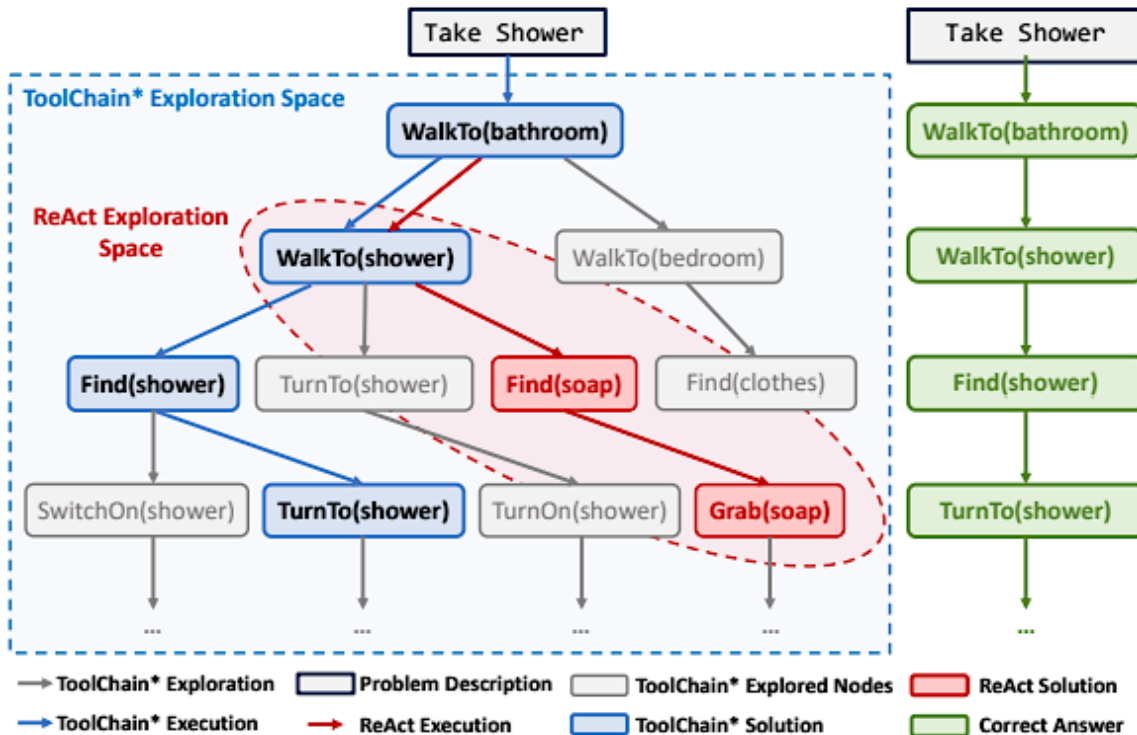
MCTS: Simulates many random rollouts to

terminal states  $Q(n, a) + c \sqrt{\frac{\log N(n)}{N(n, a)}}$

- $Q(n, a)$  average reward from history
- $\sqrt{\frac{\log N(n)}{N(n, a)}}$  encourages less-explored actions

# Reasoning & Planning Graph – Multi-Step Reasoning

## Case Study Comparison

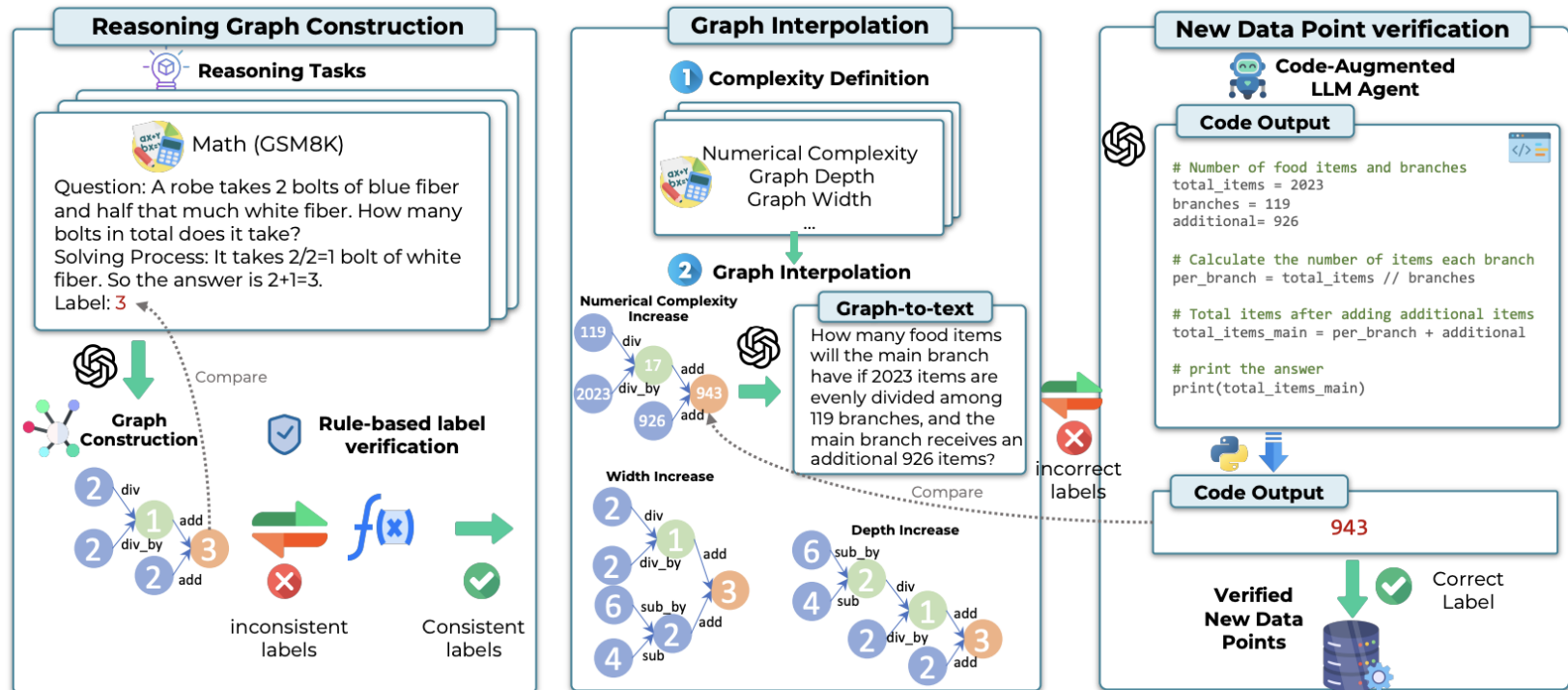


- Structured Exploration Instead of Greedy Paths
- Cost-guided Retrieval with Reasoning Flow

ToolChain\* retrieves and reasons over a dynamically growing action graph

# Reasoning & Planning Graph – Multi-Step Reasoning

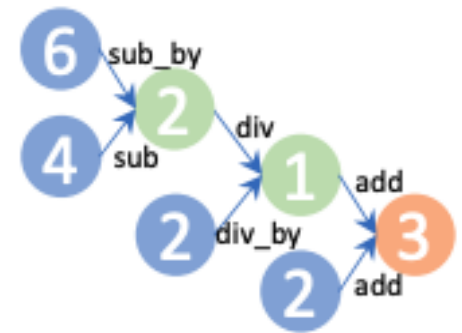
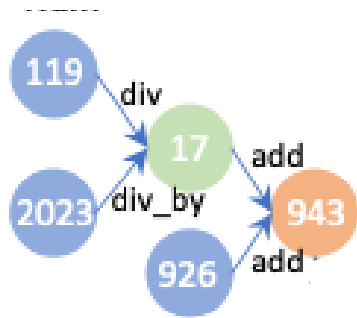
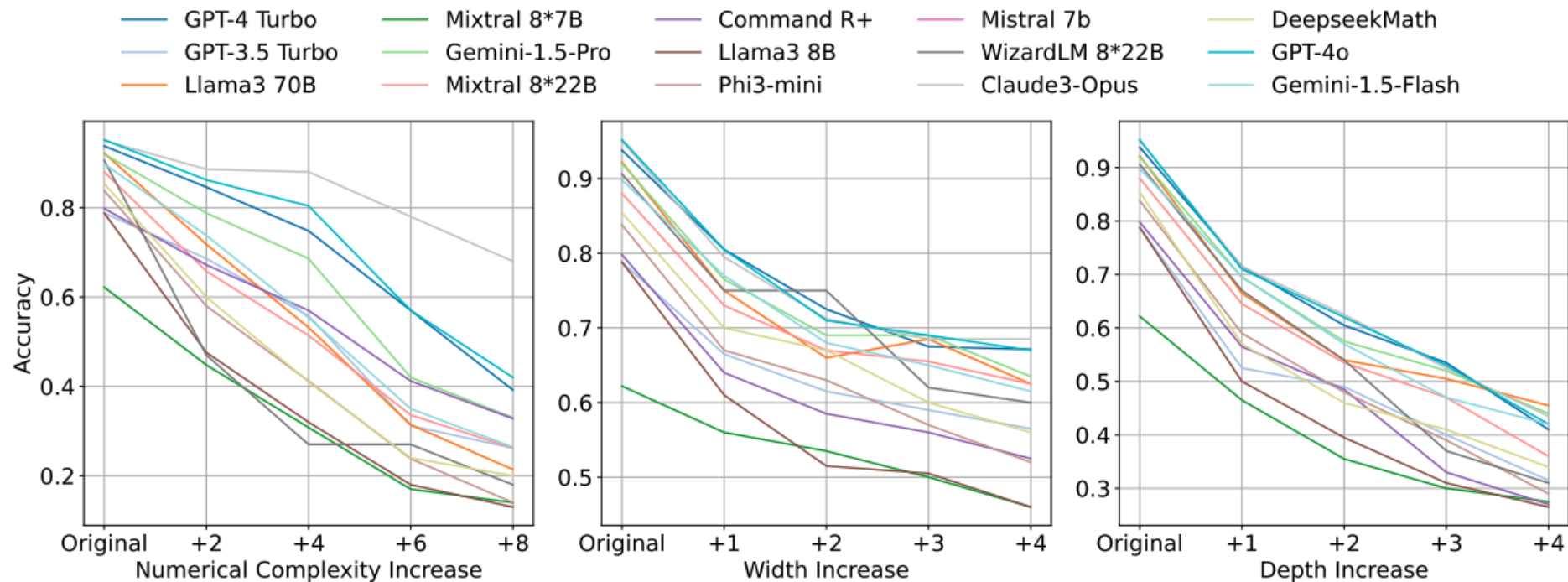
## DARG: Dynamic Evaluation via Adaptive Reasoning Graph



Reasoning graphs are powerful for reasoning ability evaluation

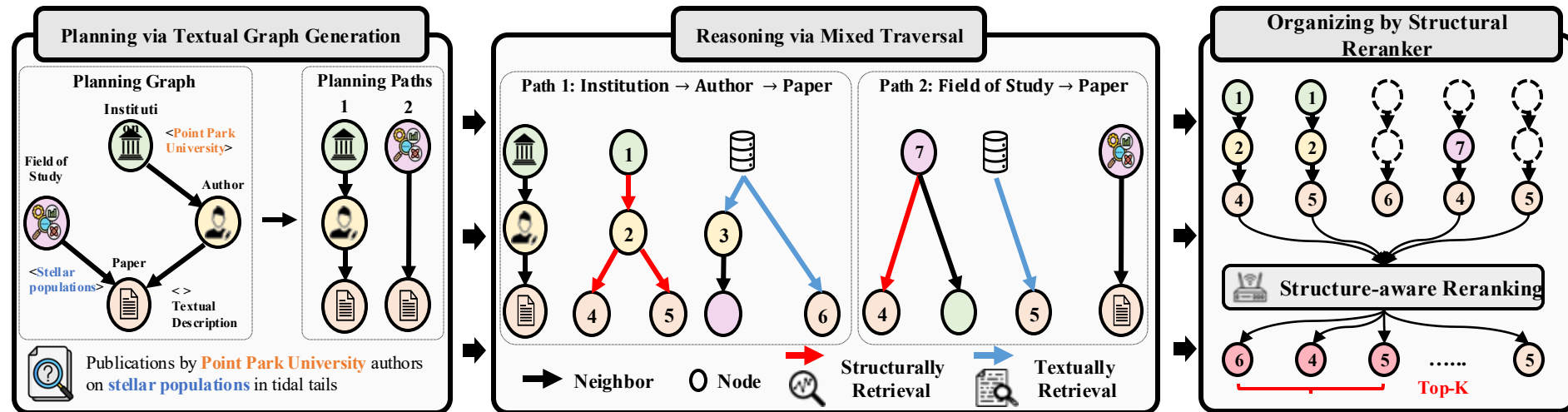
- Enable Structural Complexity Control
- Make LLM Reasoning Observable and Measurable
- Answer questions by retrieving underlying reasoning graph – Logic Fetching

# Reasoning & Planning Graph – Multi-Step Reasoning



# Reasoning & Planning Graph – Augment Retrieval Itself

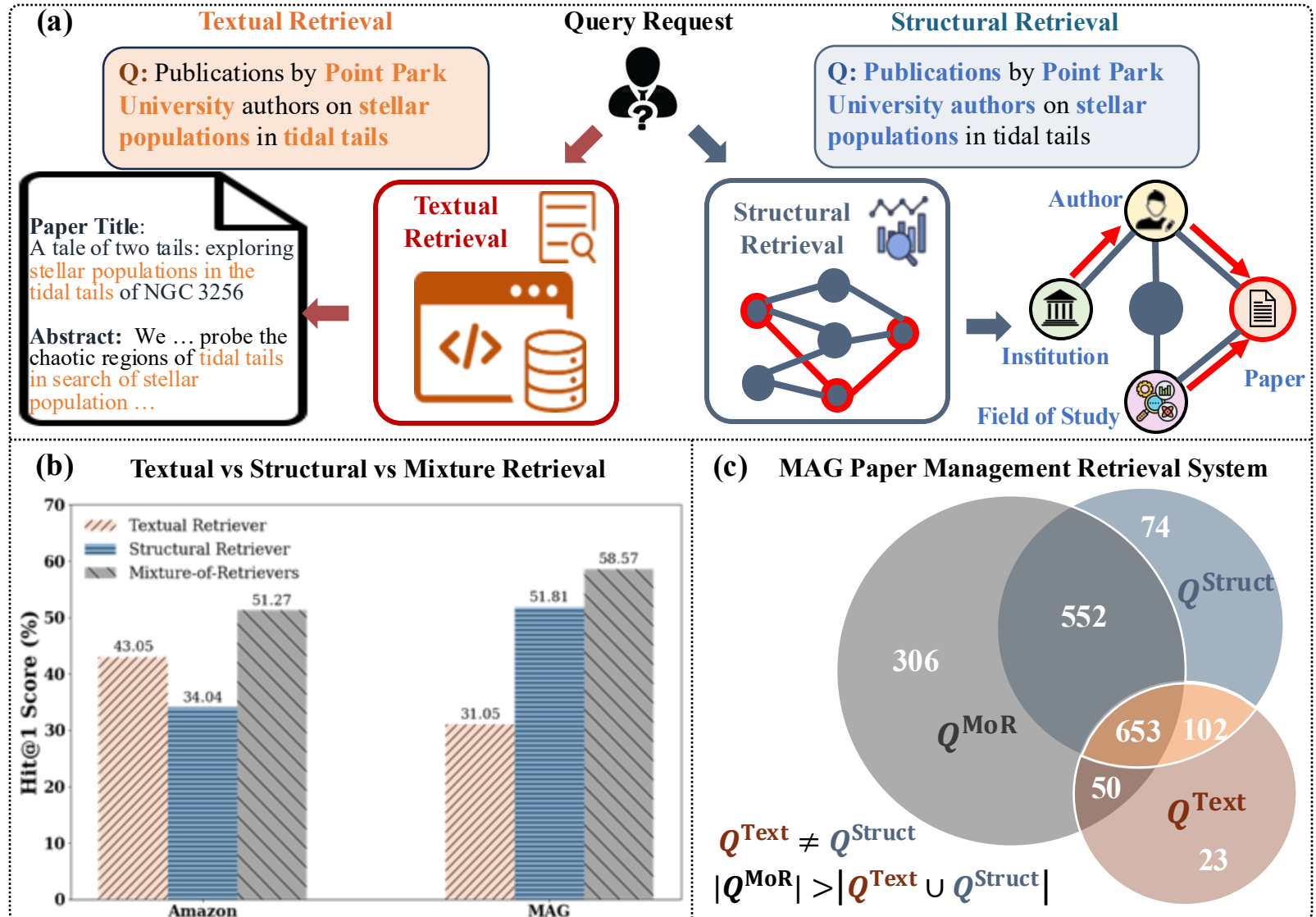
## MoR - Mixture of Structural and Textual Retrieval



- **Planning** - Given a query, generate its planning graph
- **Reasoning** - Mixed traversal guided by generated planning graph
  - Structural retrieval via graph traversal
  - Textual retrieval via textual matching
- **Organizing** - Structure-aware Rerank to select top-k candidates

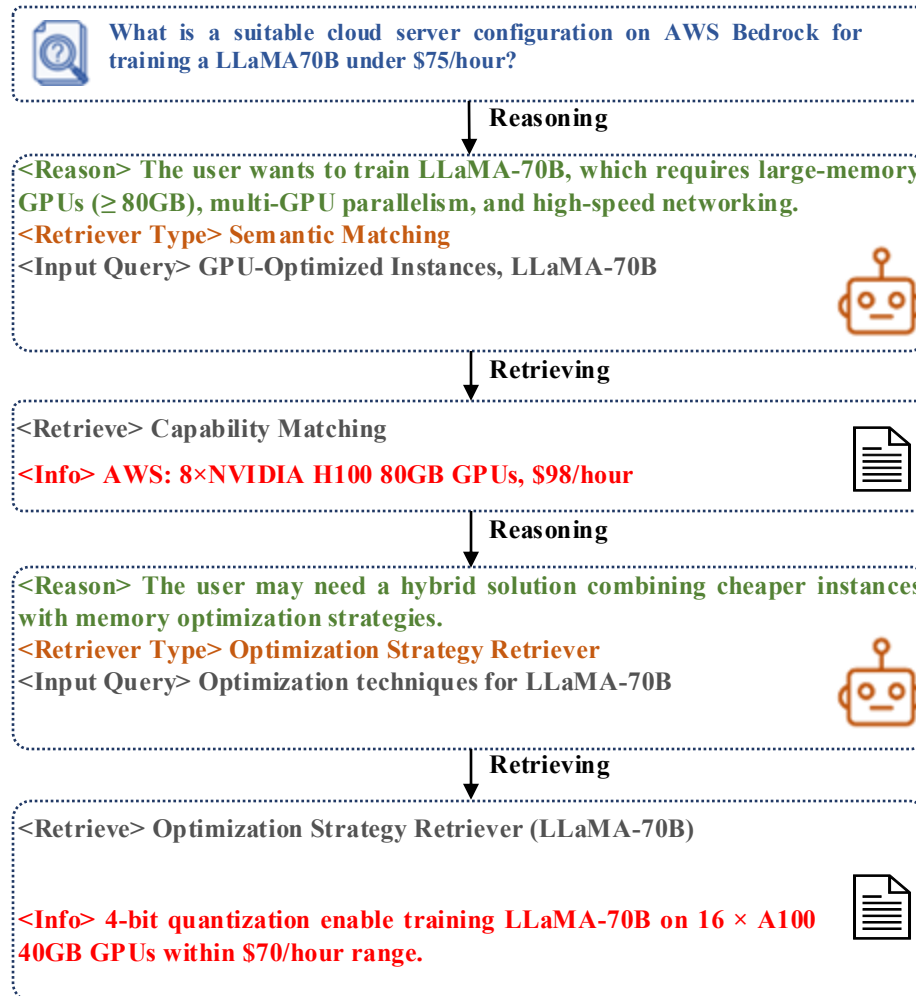


# Reasoning & Planning Graph – Augment Retrieval Itself



# Reasoning & Planning Graph – Augment Retrieval Itself

## Interleaved Reasoning and Retrieval via Reinforcement Learning



# Reasoning & Planning Graph – Augment Retrieval Itself

## Interleaved Reasoning and Retrieval via Reinforcement Learning

- Multi-turn reasoning with real-time search (<think>, <search>, <information> tokens)
- Retrieved token masking for stable RL training
- Simple outcome-based reward to supervise the reasoning + retrieval behavior.

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### Algorithm 1 LLM Response Rollout with Multi-Turn Search Engine Calls

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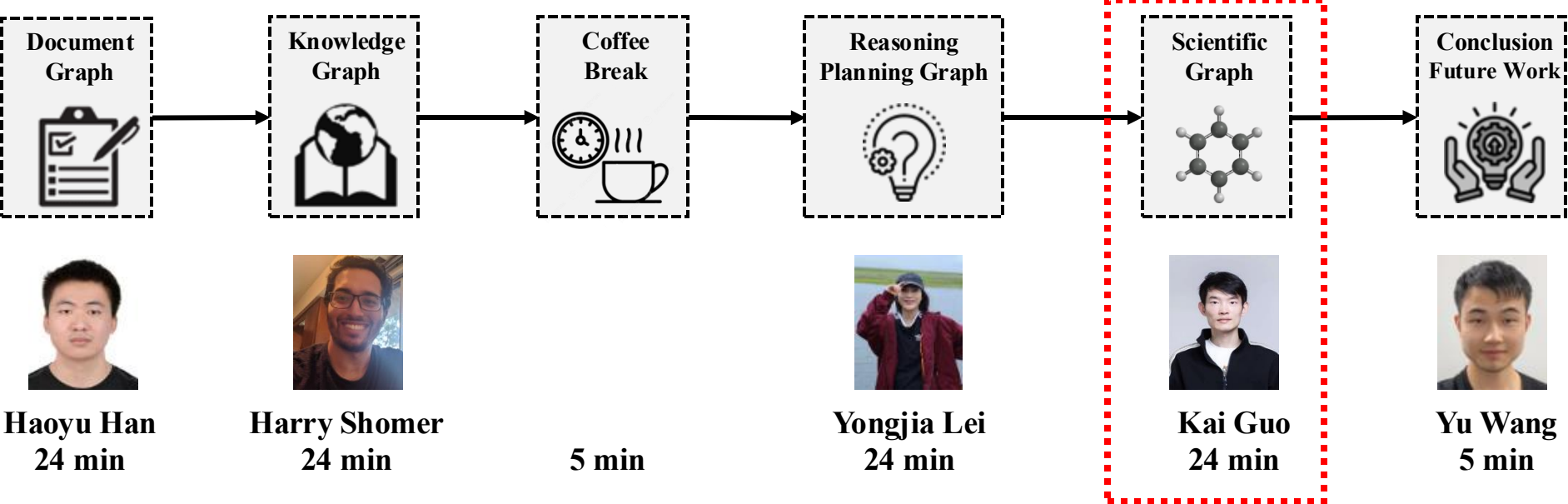
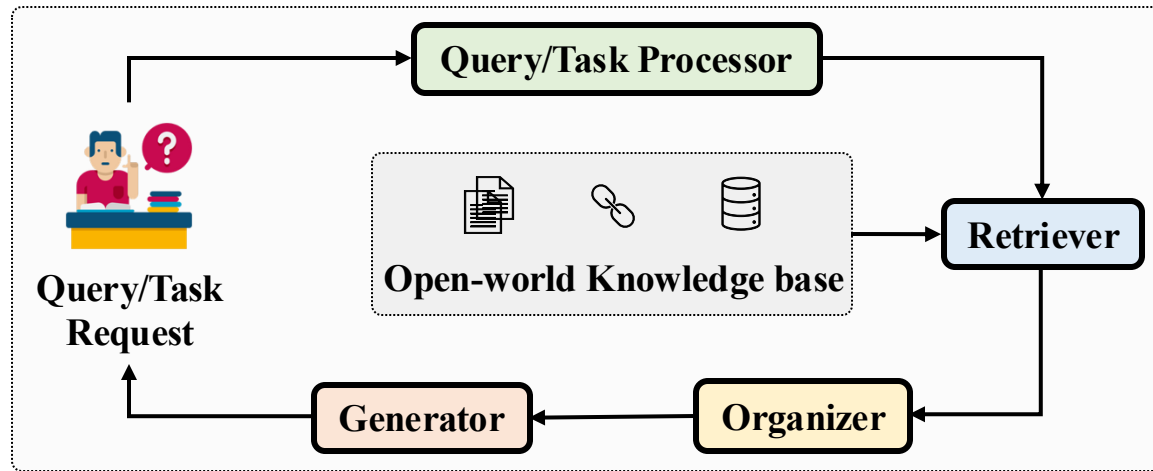
**Require:** Input query  $x$ , policy model  $\pi_\theta$ , search engine  $\mathcal{R}$ , maximum action budget  $B$ .

**Ensure:** Final response  $y$ .

```
1: Initialize rollout sequence  $y \leftarrow \emptyset$ 
2: Initialize action count  $b \leftarrow 0$ 
3: while  $b < B$  do
4:   Initialize current action LLM rollout sequence  $y_b \leftarrow \emptyset$ 
5:   while True do
6:     Generate response token  $y_t \sim \pi_\theta(\cdot \mid x, y + y_b)$ 
7:     Append  $y_t$  to rollout sequence  $y_b \leftarrow y_b + y_t$ 
8:     if  $y_t$  in [</search>, </answer>, <eos>] then break
9:   end if
10:  end while
11:   $y \leftarrow y + y_b$ 
12:  if <search> </search> detected in  $y_b$  then
13:    Extract search query  $q \leftarrow \text{Parse}(y_b, \text{<search>, </search>})$ 
14:    Retrieve search results  $d = \mathcal{R}(q)$ 
15:    Insert  $d$  into rollout  $y \leftarrow y + \text{<information>}d\text{</information>}$ 
16:  else if <answer> </answer> detected in  $y_b$  then
17:    return final generated response  $y$ 
18:  else
19:    Ask for rethink  $y \leftarrow y + \text{"My action is not correct. Let me rethink."}$ 
20:  end if
21:  Increment action count  $b \leftarrow b + 1$ 
22: end while
23: return final generated response  $y$ 
```

---

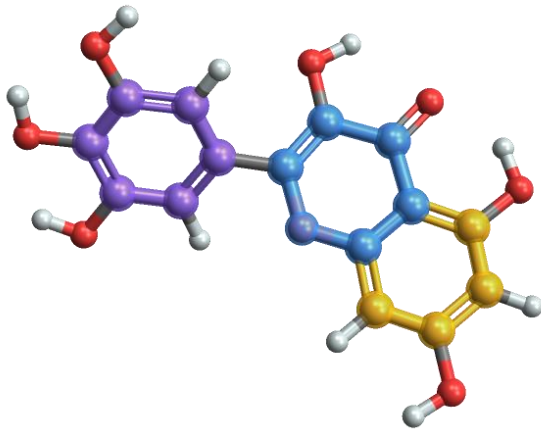
# Outline



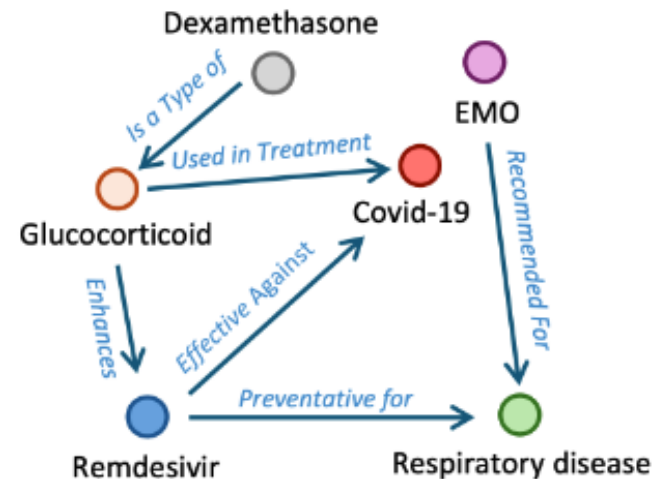
# Scientific Graph

## What is scientific graph?

Microscopic



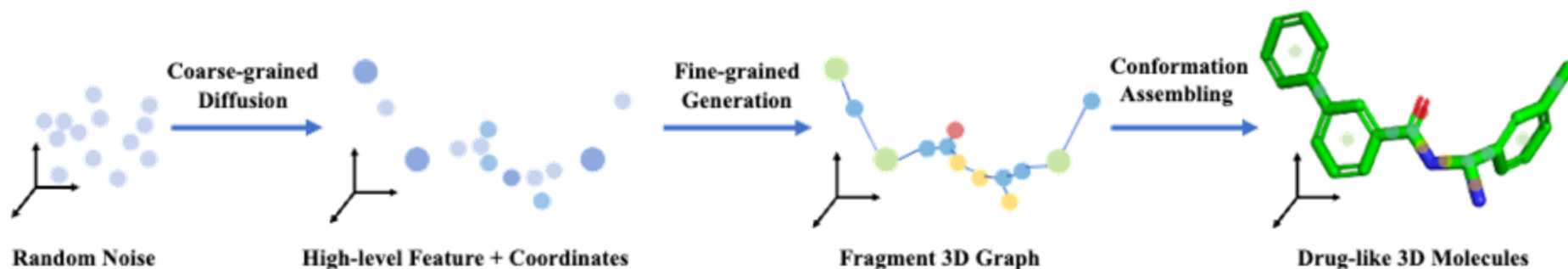
Macroscopic



## What kind of tasks can we do on scientific graph?

# Scientific Graph - Molecule Generation

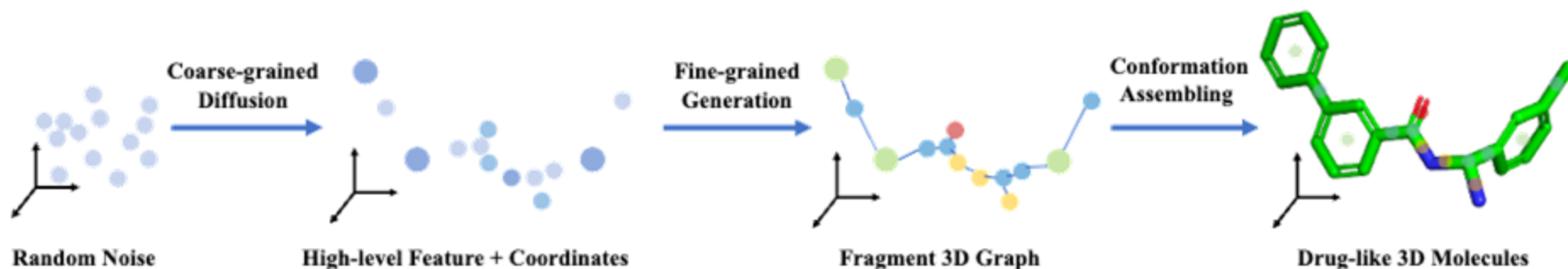
## Molecule Generation



- **Random Noise:** Initialize fragment feature vectors and 3D positions as random noise.
- **Coarse-grained Diffusion:** Diffusion-denoise fragment features and coarse 3D positions to form a high-level scaffold.
- **Fine-grained Generation:** Employ an Equivariant GNN with iterative refinement to predict fragment bonds and precise atomic coordinates.
- **Conformation Assembling:** Assemble fragments into a complete 3D molecule.

# Scientific Graph - Molecule Generation

## Why GraphRAG for Molecule Generation?



- **Slow, resource-heavy generation:** Efficient generation guided by retrieved high-performing exemplar molecules.
- **Lack of prior chemical knowledge:** Introduce real molecules or fragments as structural priors to improve generation quality.
- **Lack of controllability:** Guide the generation direction precisely based on retrieved molecules with desired properties.



# Scientific Graph - Molecule Property Prediction

## Molecule Property Prediction

Molecule property prediction is the task of using LLMs to predict a molecule's chemical properties from its structural representation.

**Instruction:** Lumo is the lowest unoccupied molecular orbital energy.

**What's the Lumo value of this molecule?**

**Molecule SMILES:** CCC(O)CN(C)C=O



**Answer:** 0.03eV

**SMILES** is a textual encoding of molecules topology, such as atom types, bond types, and branching

# Scientific Graph - Molecule Property Prediction

## Why GraphRAG for Molecule Property Prediction?

**Instruction:** The assay is PUBCHEM-BIOASSAY:  
NCI human tumor cell line growth inhibition assay.

**Question:** Is this molecule effective to this assay?

**Input:** CNC=O



Answer: Yes



**Instruction:** The assay is PUBCHEM-BIOASSAY:  
NCI human tumor cell line growth inhibition assay. Here  
are some examples.

**Examples:**

CC(C)C(N)=O No

O=CNC=Cc1ccccc1 No

**Question:** Is this molecule effective to this assay?

**Input:** CNC=O

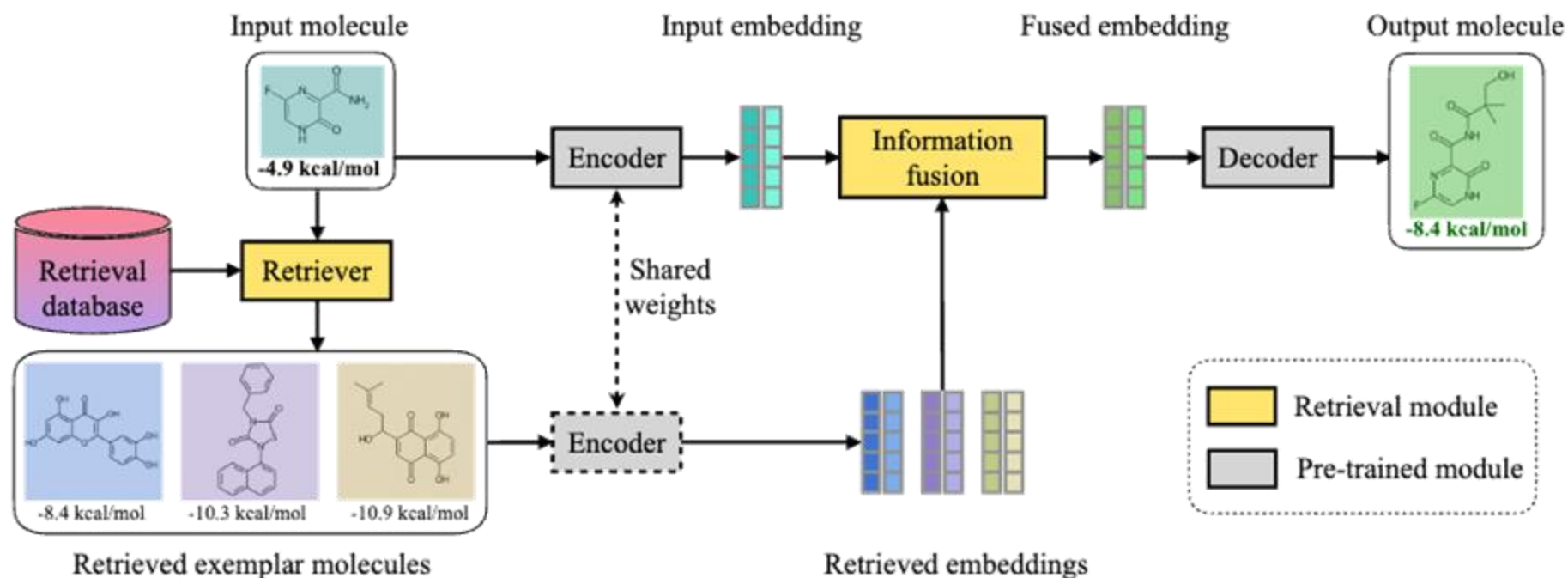


Answer: No



By retrieving exemplar molecules **structurally similar** to CNC=O as demonstration and including them in the prompt, the LLM can make accurate predictions.

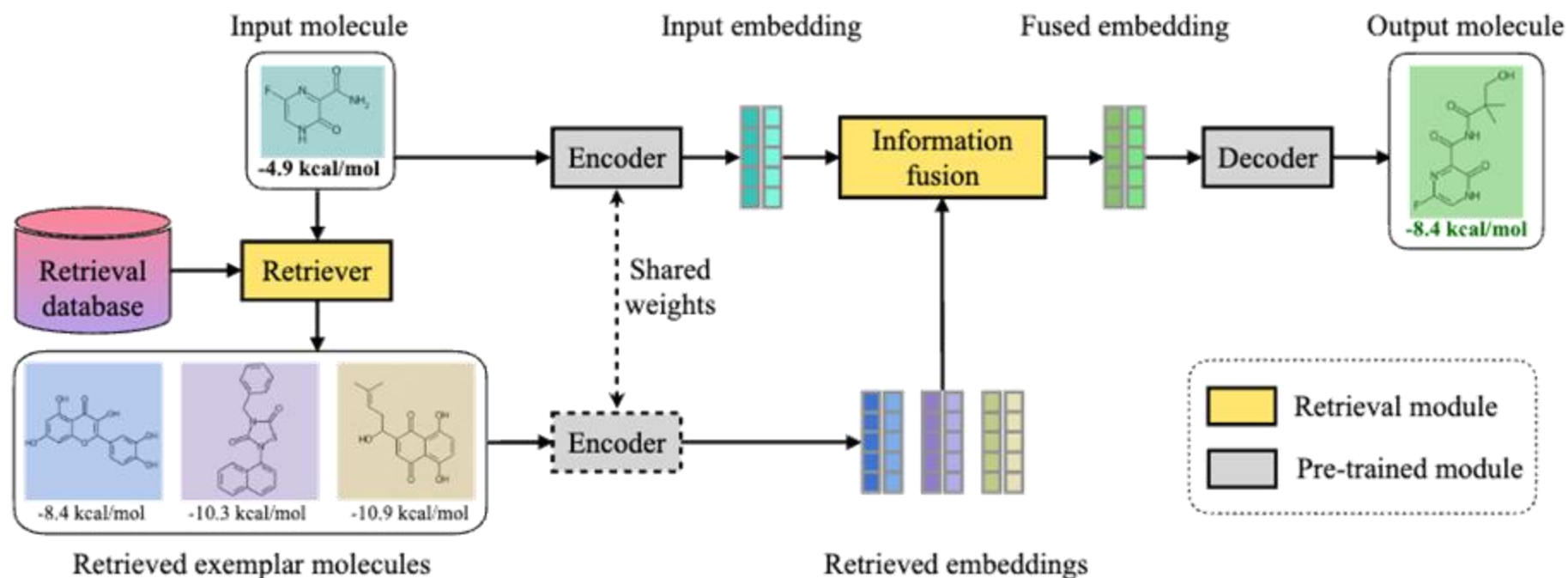
# Scientific Graph - Molecule Generation



**Main problem:** Data is scarce and Molecular Property Control is Difficult

**Core idea:** Retrieve a set of exemplar molecules to guide the generation model.

# Scientific Graph - Molecule Generation

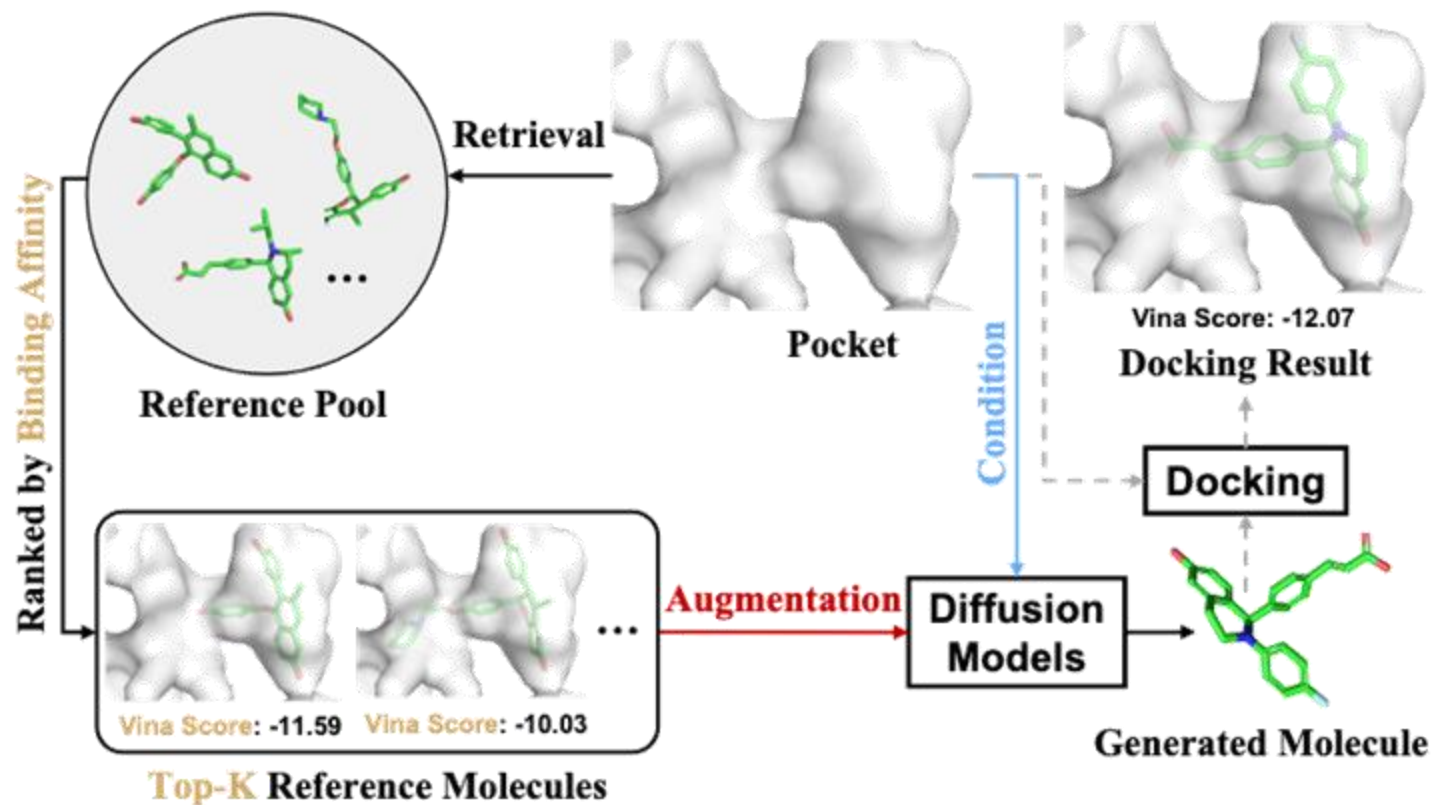


**Retrieval Database:** Collect exemplar molecules with desired properties.

**Molecule Retrieval:** Property filtering, then select top-K similar molecules using KNN.

**Information Fusion:** Use cross-attention to fuse input and exemplar embeddings for molecule generation via a pre-trained transformer-based model.

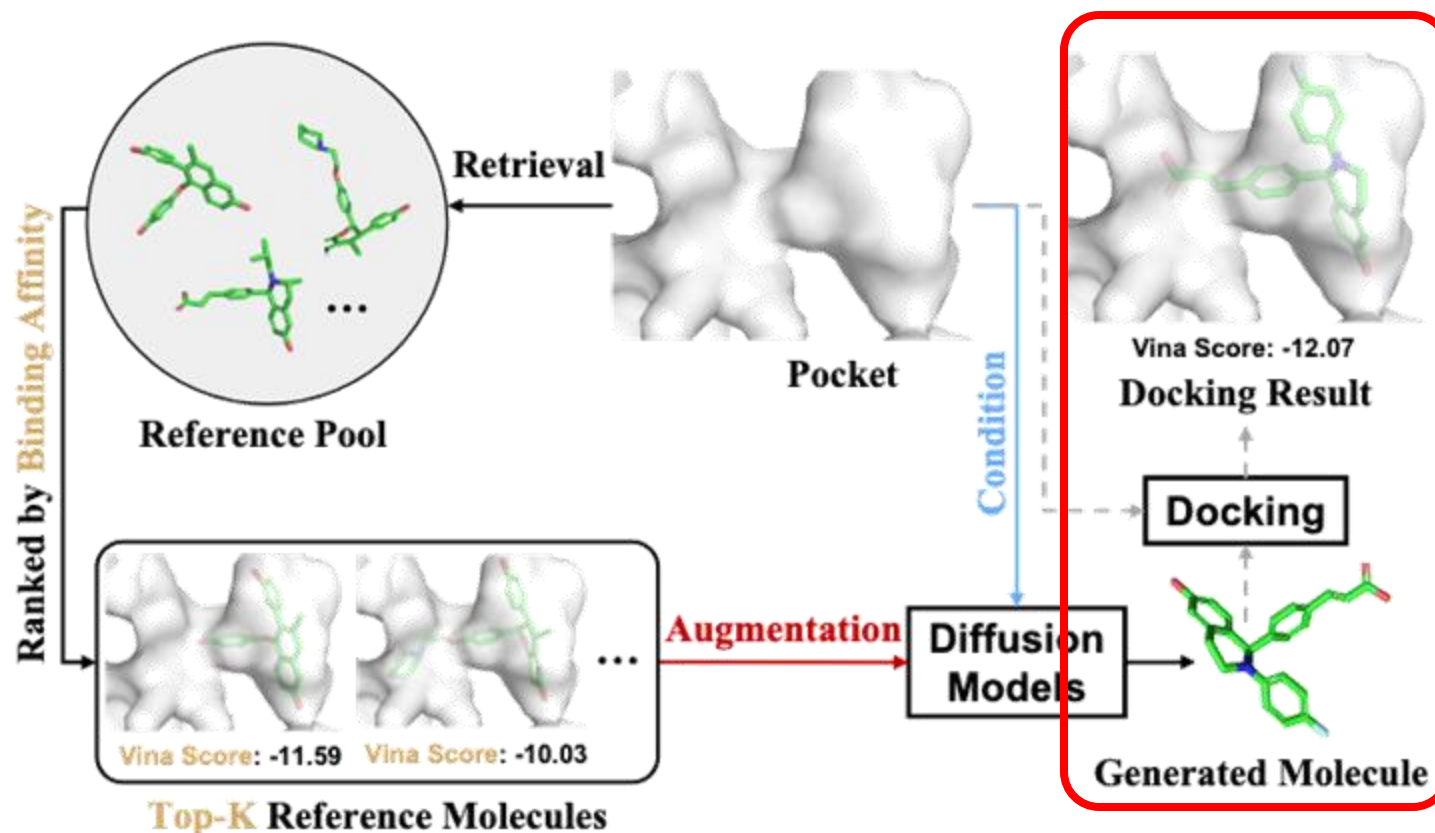
# Scientific Graph - Molecule Generation



**Main problem:** Molecule generation without target awareness → poor binding.

**Core idea:** Retrieve binding-aware references → guide diffusion to generate target-specific, high-affinity molecules.

# Scientific Graph - Molecule Generation

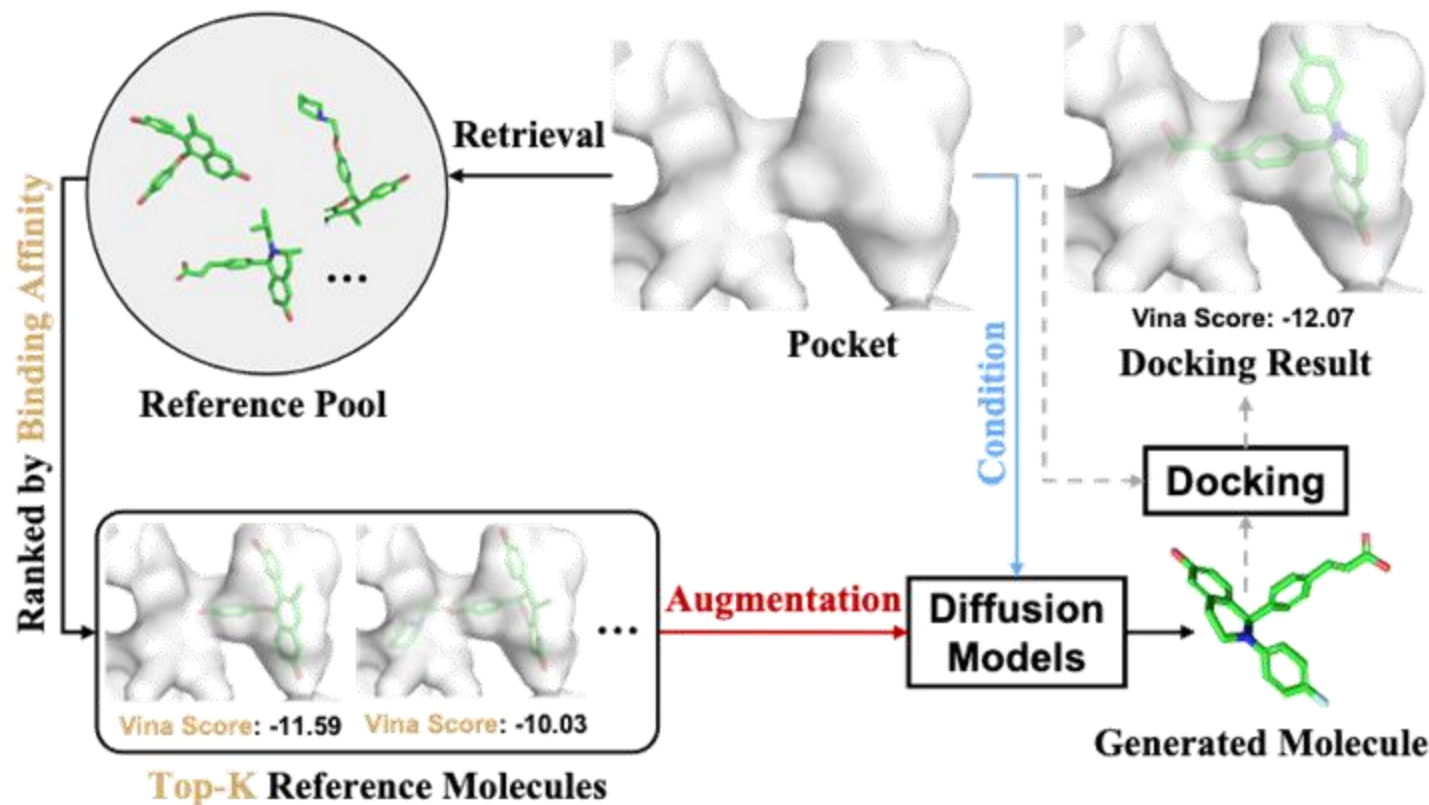


## What is docking?

Predict and select small **molecules** that can **effectively bind** to **disease-related protein targets**.

**Starting points** for further optimization toward the development of drug candidates.

# Scientific Graph - Molecule Generation

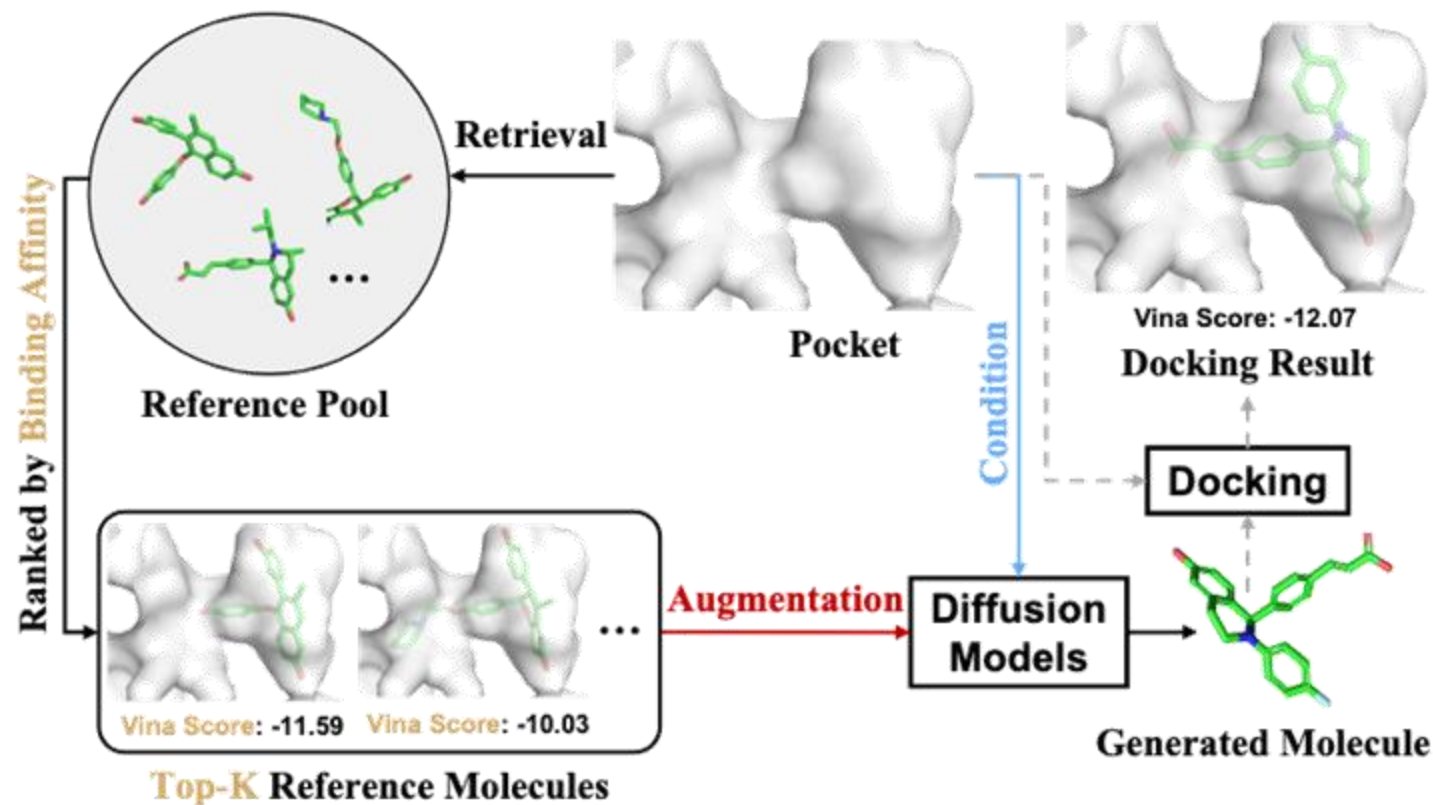


## Why use graph-based retrieval?

- Ignore target protein structure → Poor binding when evaluated by docking.
- Retrieve strong-binding reference molecules → Guide diffusion model → Generate protein-specific, high-affinity molecules.



# Scientific Graph - Molecule Generation



## How to retrieve reference molecules?

- Target Pocket Encoding
- Precompute Reference Pool
- Similarity Search (L2 Distance)
- Retrieve Top-K Molecules
- Use for Generation

# Scientific Graph - Molecule Property Prediction

## Zero-shot Instruction

**Instruction:** Lumo is the lowest unoccupied molecular orbital energy. What's the Lumo value of this molecule?  
**Input:** CCC(O)CN(C)C=O

## Few-shot Instruction

**Instruction:** The assay is PUBCHEM\_BIOASSAY: NCI human tumor cell line growth inhibition assay ... Here are some examples.

**SMILES:** CC(C)C(N)=O

**label:** No

**SMILES:** O=CNC=Cc1ccccc1

**label:** No

**SMILES:** COC(=O)C#CC(N)=O

**label:** No

...

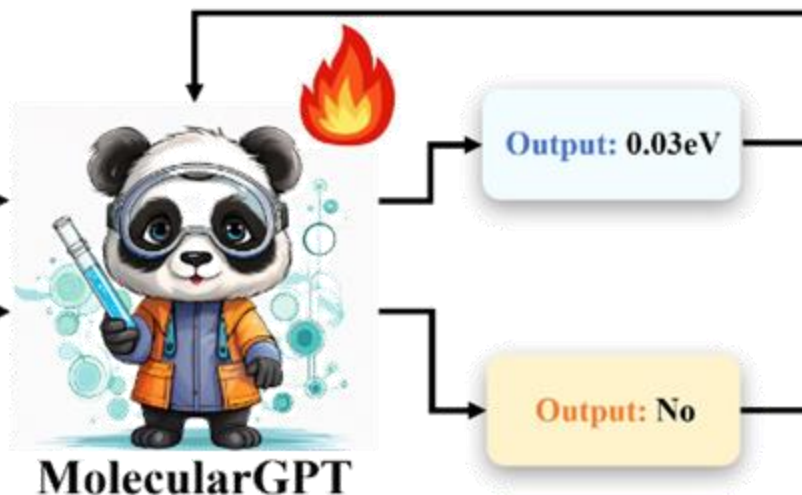
Is this molecule effective to this assay?

**Input:** CNC=O

Structure-aware  
Demonstrations

Similarity  
decreasing

## Hybrid Instruction Tuning



## Multi-domain properties



Chemichysics



Toxicity



Pharmacokinetics



Bio-activity

**Main problem:** LLMs lack domain-specific Knowledge

**Core idea:** MolecularGPT retrieve relevant molecules based on structure to enhance LLM.

# Scientific Graph - Molecule Property Prediction

## Zero-shot Instruction

**Instruction:** Lumo is the lowest unoccupied molecular orbital energy. What's the Lumo value of this molecule?  
**Input:** CCC(O)CN(C)C=O

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**SMILES:** CC(C)C(N)=O

**label:** No

**SMILES:** O=CNC=Cc1ccccc1

**label:** No

**SMILES:** COC(=O)C#CC(N)=O

**label:** No

...

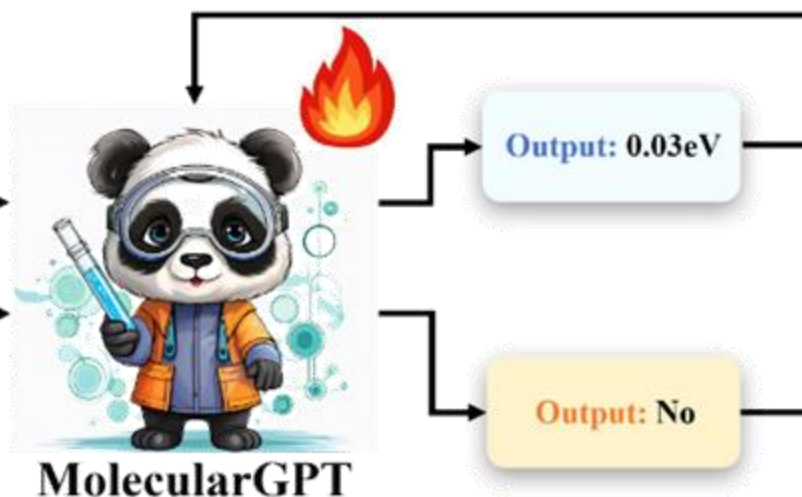
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**Input:** CNC=O

Structure-aware  
Demonstrations

Similarity  
decreasing

## Hybrid Instruction Tuning



## Multi-domain properties



Chemcophysics



Toxicity



Pharmacokinetics



Bio-activity

**Data Preparation:** Collect (molecule, property) pairs

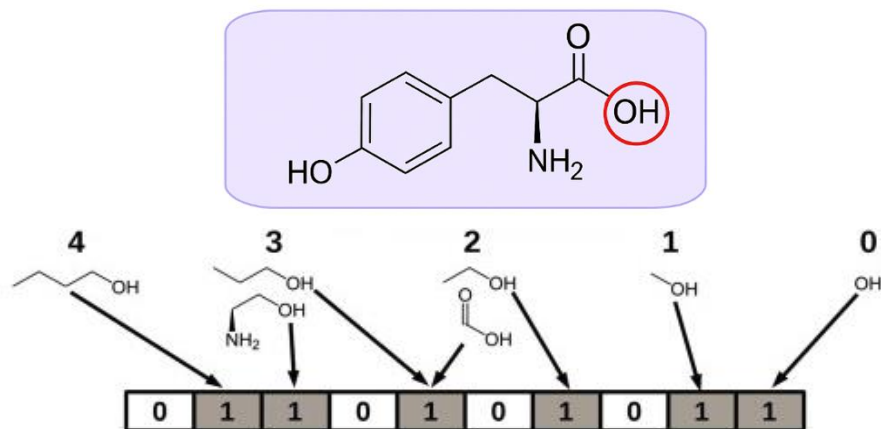
**SMILES Conversion:** Represent molecules as SMILES strings for input.

**Neighbor Retrieval:** Tanimoto similarity

# Scientific Graph - Molecule Property Prediction

## What is Tanimoto similarity?

A similarity metric between two binary fingerprints A and B



$$\text{Tanimoto}(A, B) = \frac{|A \cap B|}{|A| + |B| - |A \cap B|}$$

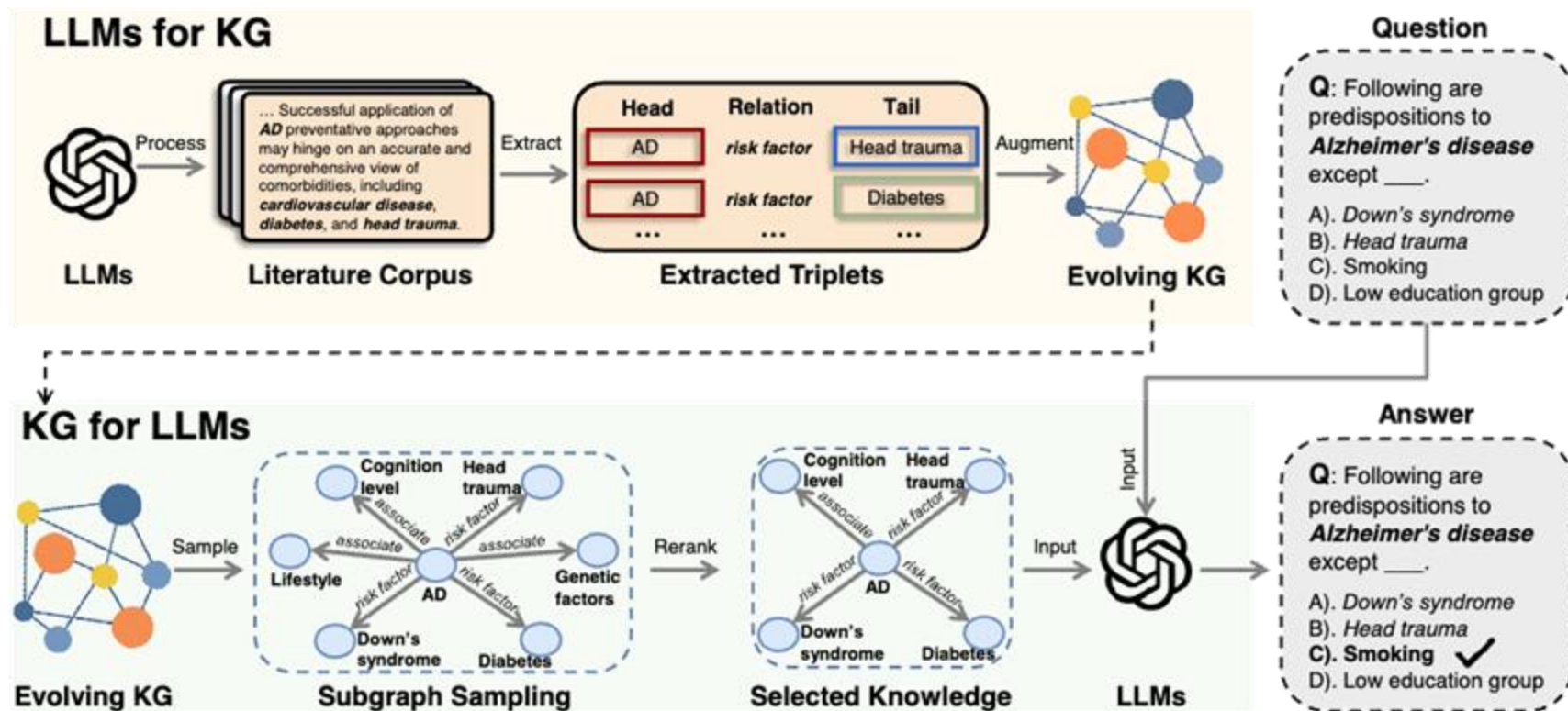
**Data Preparation:** Collect (molecule, property) pairs

**SMILES Conversion:** Represent molecules as SMILES strings for input.

**Neighbor Retrieval:** **Tanimoto similarity**



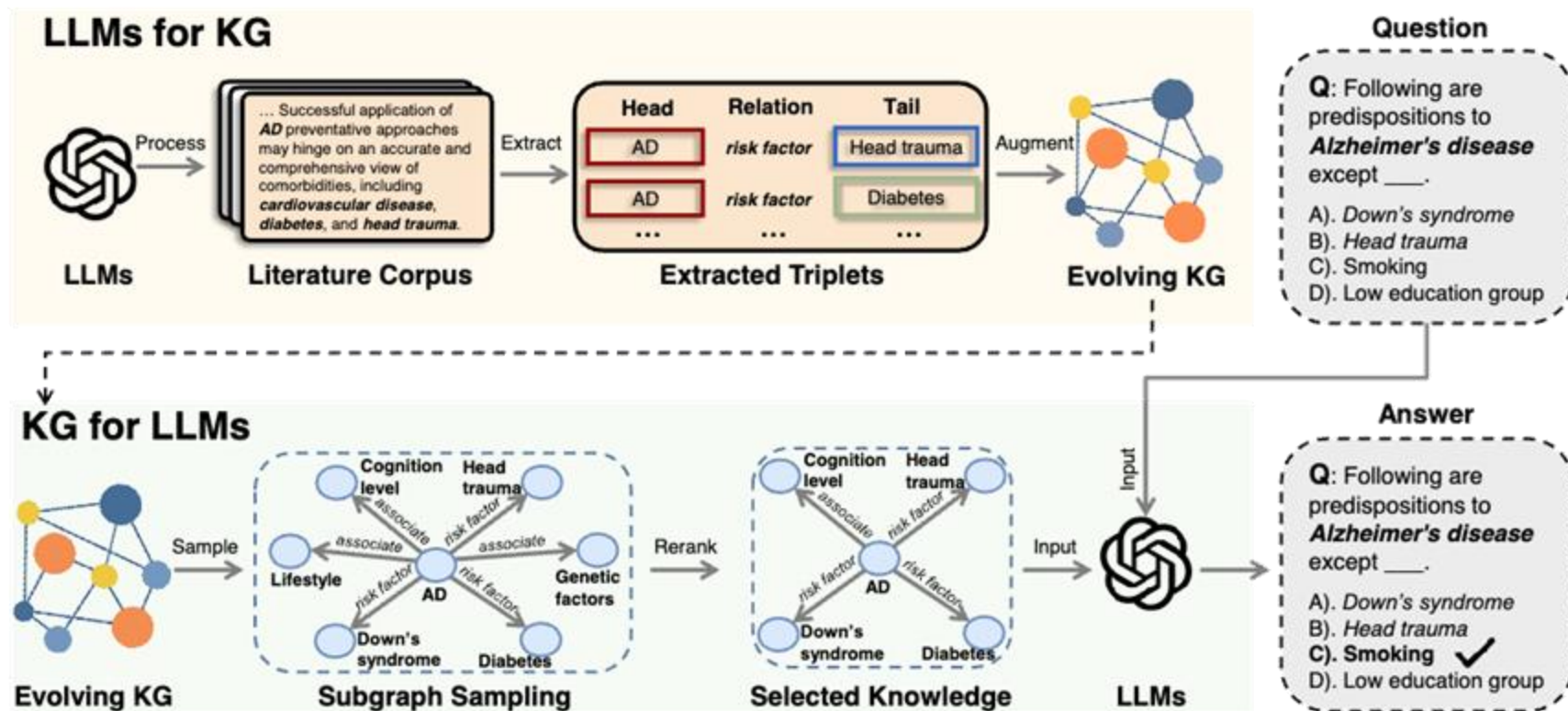
# Scientific Graph - Question Answering



**Main problem:** LLMs struggle to answer Alzheimer's Disease (AD) questions due to limited integration of specialized biomedical knowledge.

**Core idea:** DALK augments LLMs with a scientific literature-derived knowledge graph to improve reasoning on AD-related questions.

# Scientific Graph - Question Answering



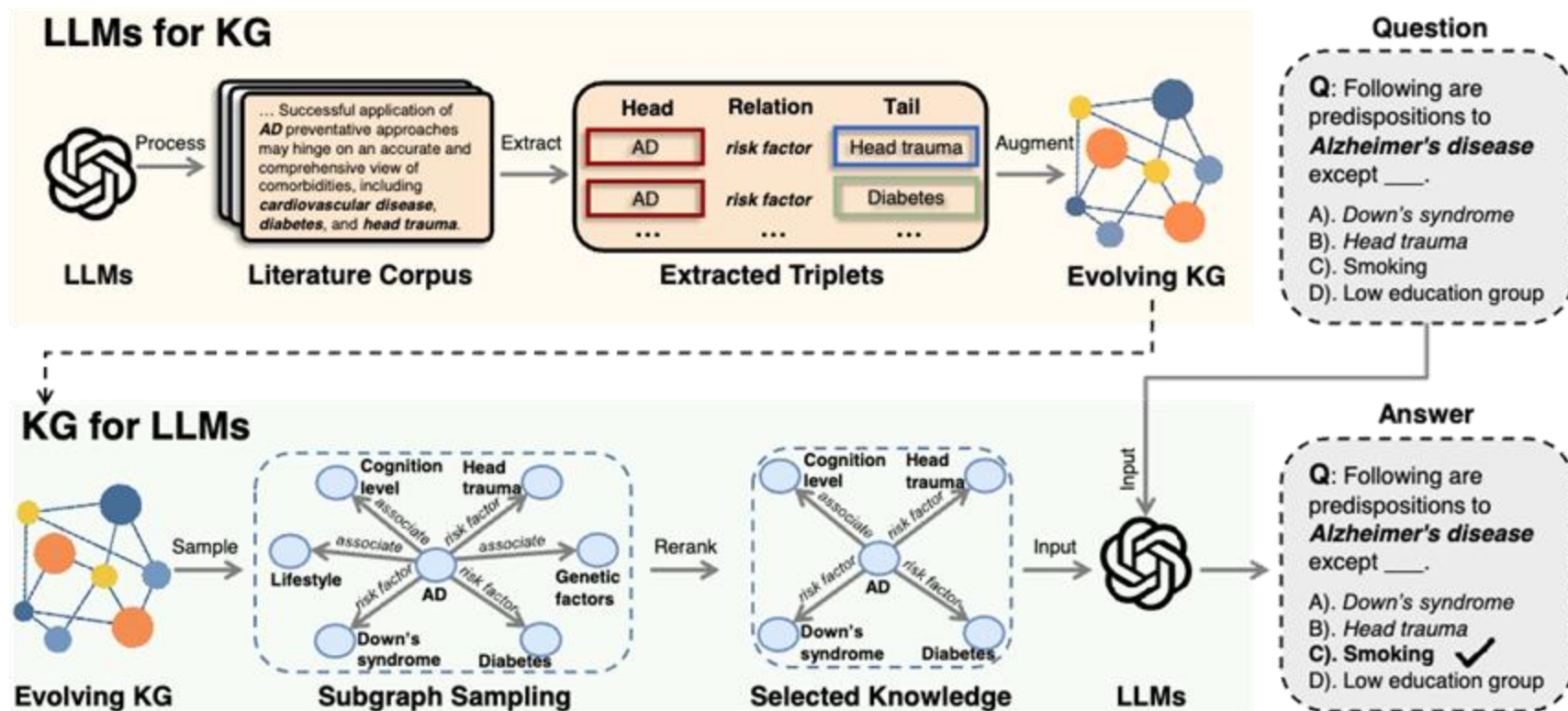
**Entity Recognition:** Use [PubTator Central](#) to identify biomedical entities.

**Relation Extraction:**

- Pairwise: LLMs describe pairwise relations.
- Generative: LLMs generate all triplets.

**Evolving KG:** Update KG to reflect new discoveries annually

# Scientific Graph - Question Answering



**Entity Extraction and Linking for query**

**Path Exploration:** K-hop path triplets of seeding nodes and their induced subgraph

**Neighbor Exploration:** Neighbor of seeding nodes and their induced subgraph



# Scientific Graph - Future Direction

## Multi-modal GraphRAG for Scientific Graph

**Motivation:** Scientific data is inherently multi-modal:

- **Text** (Papers, Document)
- **Image** (Medical Images: MRI and CT)
- **Table**

Current GraphRAG mainly focus on text and structure separately.

# Scientific Graph - Future Direction

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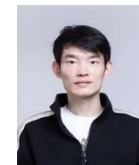
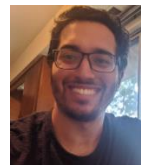
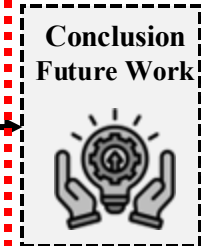
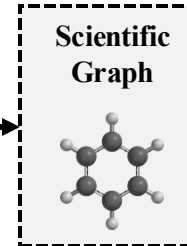
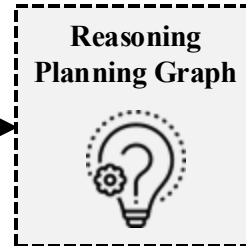
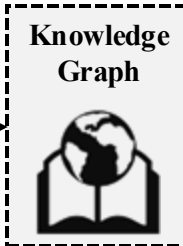
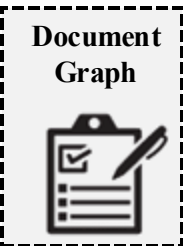
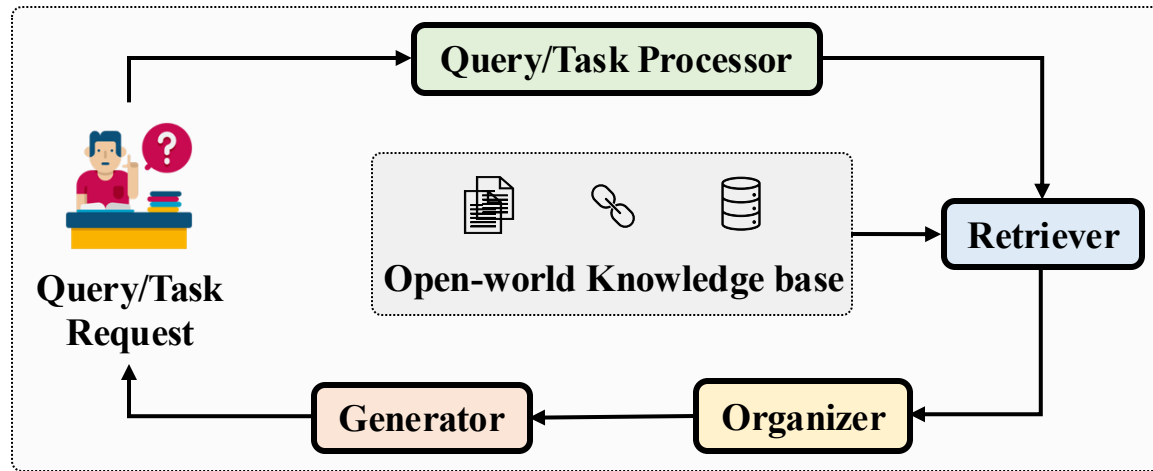
## **Towards Trustworthy GraphRAG for Scientific Graphs**

**Motivation:** GraphRAG has been really deployed in many high-stake scenarios

- **Retrieval focuses on associative facts, not verified causal relations**
- **Generated answers lack scientific rigor and are less trustworthy**

Building Causal Evidence Rule-based Retrieval-augmented Generation

# Outline



Haoyu Han  
24 min

Harry Shomer  
24 min

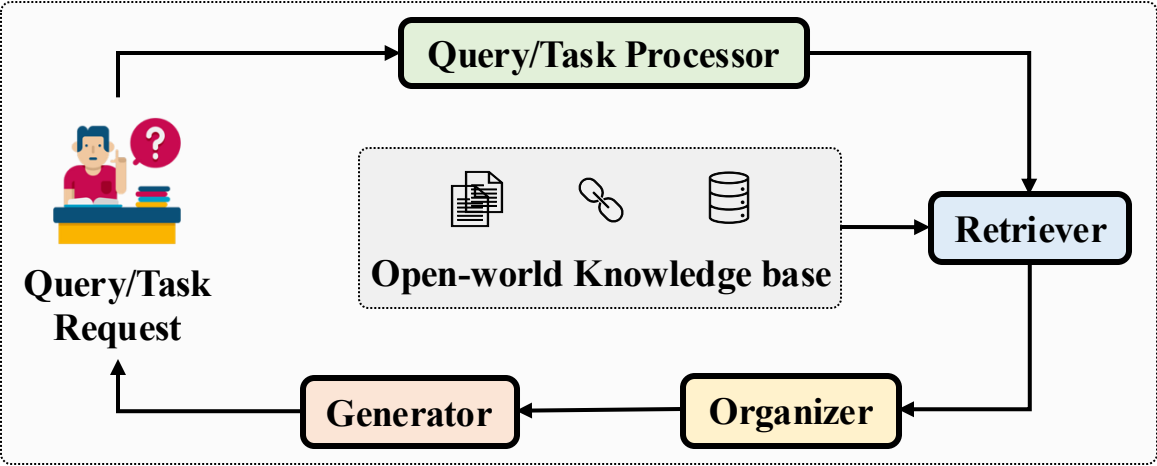
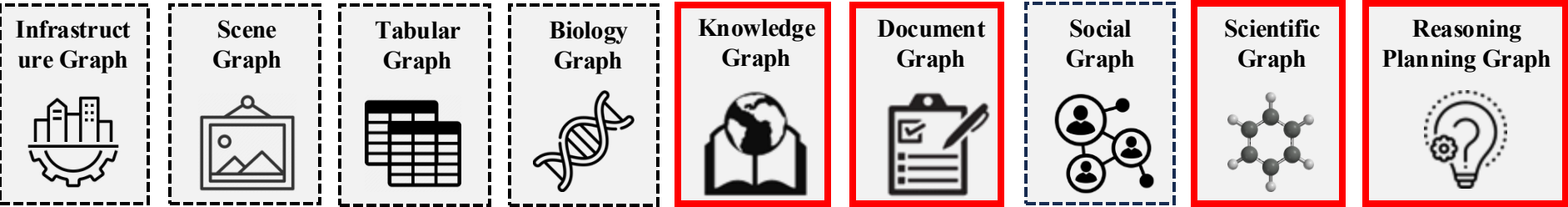
4 min

Yongjia Lei  
24 min

Kai Guo  
24 min

Yu Wang  
5 min

# Conclusion



<https://github.com/Graph-RAG/GraphRAG/>

Name Entity Recognition
Relational Extraction
Query Structuration
Query Decomposition
Query Expansion

Heuristic-based	Learning-based
Entity Linking	Shallow Embedding
Relational Matching	Deep Embedding
Graph Traversal	Advanced
Graph Kernel	Integrated
Domain Expertise	Iterative
	Adaptive

Reranking	Verbalization
Pruning	Linear-based
Semantic-based	Template-based
Syntactic-based	Augmentation
Structure-based	Structure
Dynamic	Feature

Prediction-based
LLM-based
Verbalizing
Embedding-fusion
Positional Embedding-fusion
Graph-based

Graph Construction
Explicit Construction
Implicit Construction



# Future Work 1 – GraphRAG on other domains

Infrastructure Graph



Scene Graph



Tabular Graph



Biology Graph



Knowledge Graph



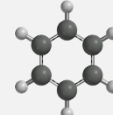
Document Graph



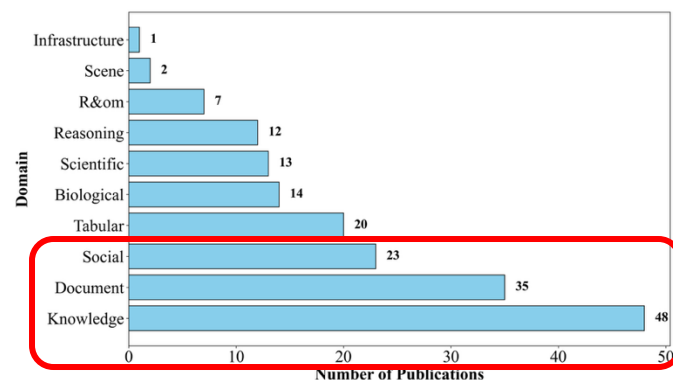
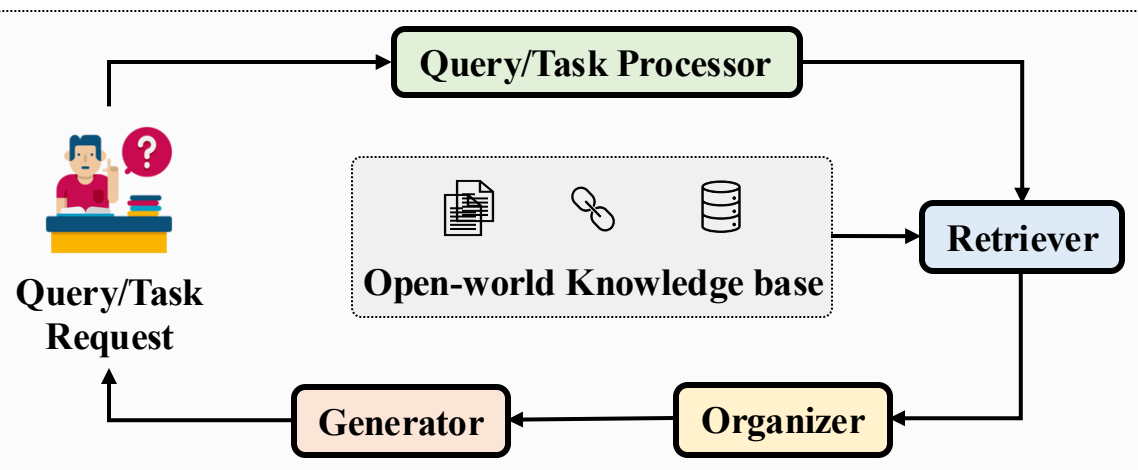
Social Graph



Scientific Graph



Reasoning Planning Graph



Statistics surveyed until 12/31/2024

Name Entity Recognition
Relational Extraction
Query Structuration
Query Decomposition
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Prediction-based
LLM-based
Verbalizing
Embedding-fusion
Positional Embedding-fusion
Graph-based

Graph Construction
Explicit Construction
Implicit Construction

# Future Work 2 – GraphRAG Module Design

- **Query Preprocessor** – Analyze Query Structure and Topology

- **Retriever**

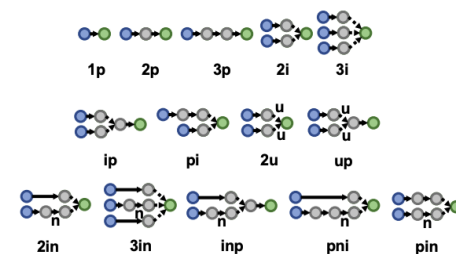
- Harmonizing Internal and External Knowledge
- How to embedding different types of structured knowledge (e.g., cluster vs path)
- Reasoning, planning, and thinking along the way (e.g., Search-R1)

- **Organizer**

- Retrieved Graph can be large, balancing completeness and conciseness (e.g., exponentially growth receptive field)
- Optimal Data Structuring that generator can leverage
- Align retrieved resources from different parties (e.g., multi-modality graph)

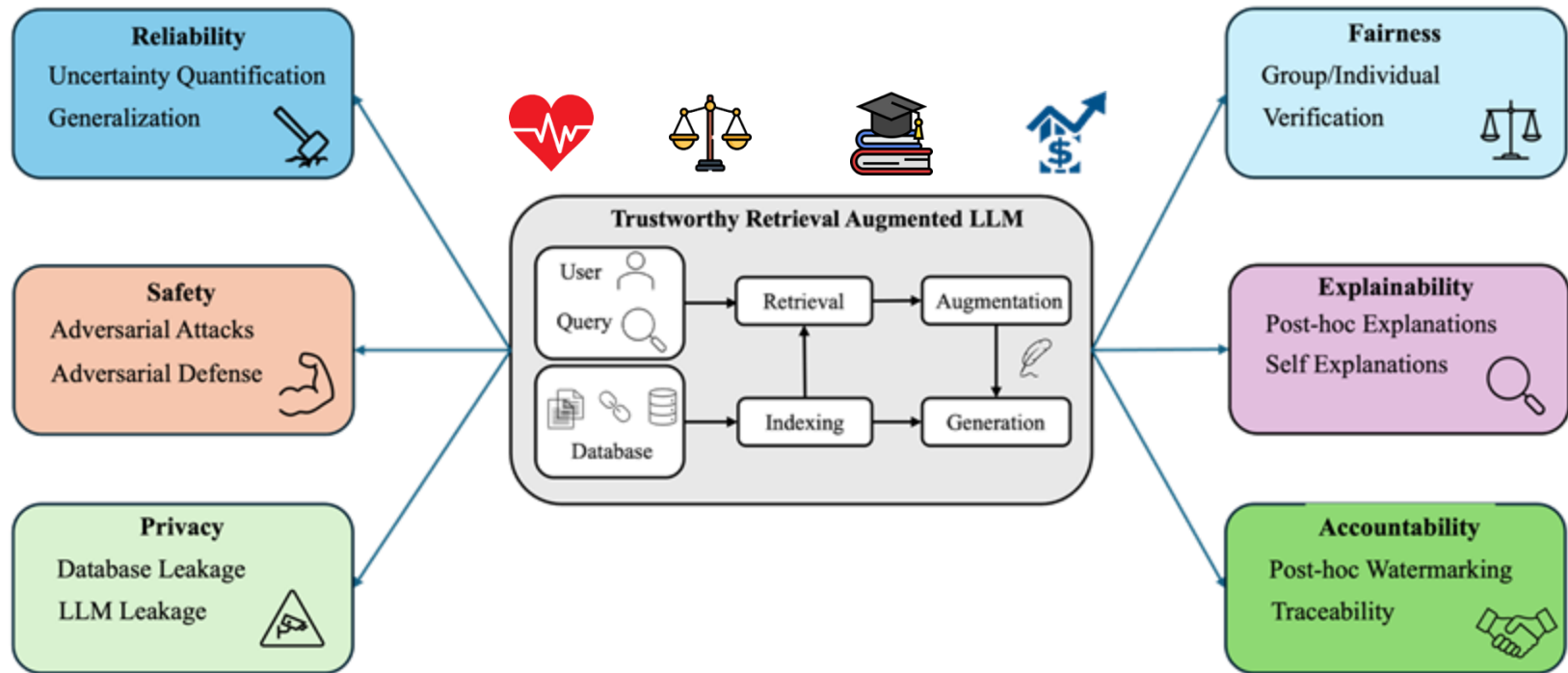
- **Generator**

- Correct Format of Prompting (e.g., adjacent list, markdown format, .....)
- Structural Encoding for expressing the graph structure



[Ren et al](#)

# Future Work 3 – Trustworthy GraphRAG

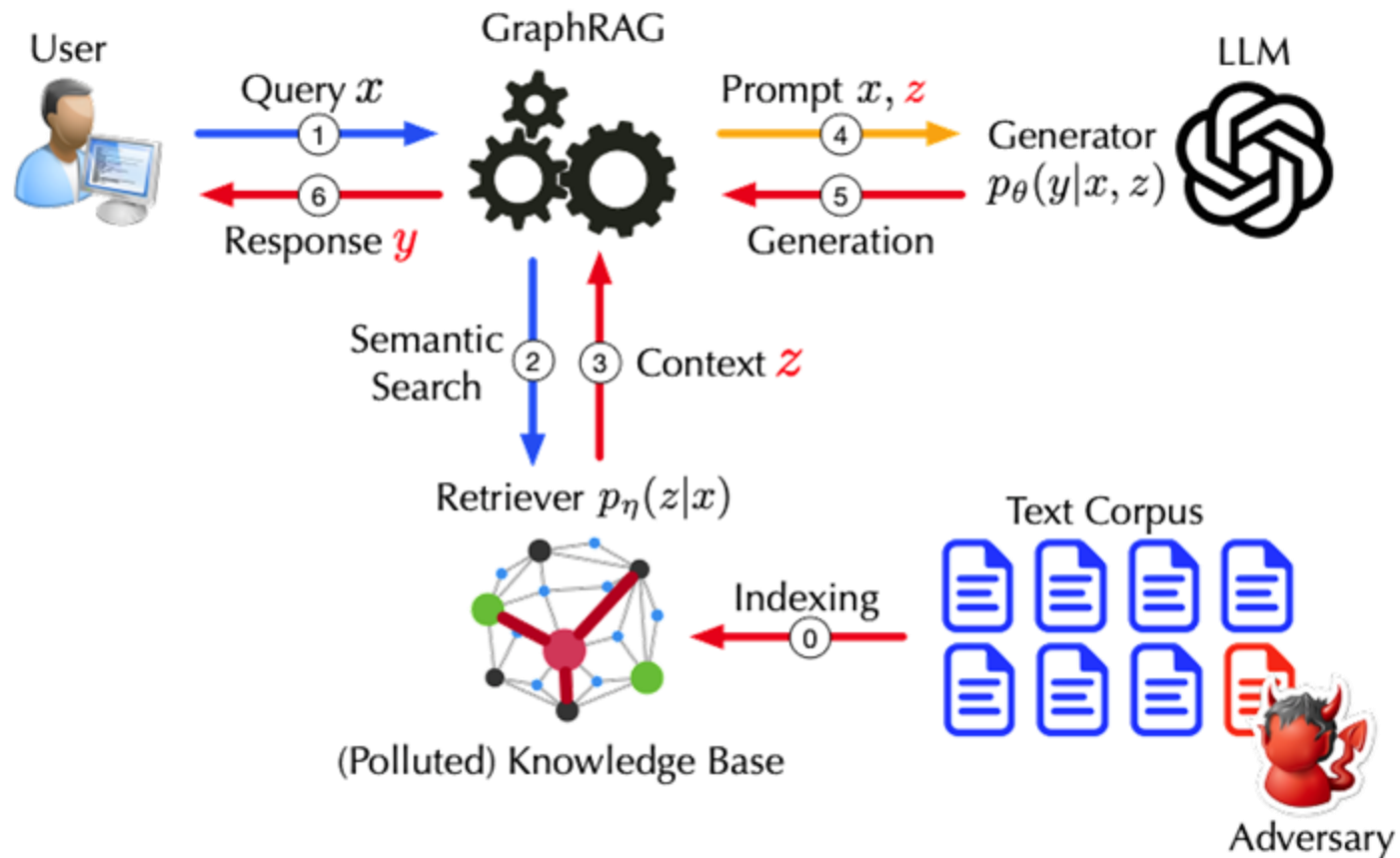


How about the unique trustworthy challenges caused graph structure?

<https://github.com/Arstanley/Awesome-Trustworthy-RAG>



# Future Work 3 – Trustworthy GraphRAG



**How about the unique trustworthy challenges caused graph structure?**

<https://github.com/Arstanley/Awesome-Trustworthy-RAG>

# Future Work 4 – Data-centric GraphRAG

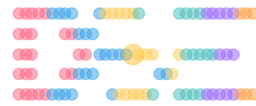
- **Balance Internal and External Knowledge**



- **Trade-off Among Accuracy, Diversity, and Novelty**



# Thank you for your listening!



## Retrieval-Augmented Generation with Graphs (GraphRAG)

Haoyu Han<sup>1</sup>, Yu Wang<sup>2</sup>, Harry Shomer<sup>1</sup>, Kai Guo<sup>1</sup>, Jiayuan Ding<sup>2</sup>, Yongjia Lei<sup>2</sup>, Mahantesh Halappanavar<sup>3</sup>, Ryan A. Rossi<sup>4</sup>, Subhabrata Mukherjee<sup>5</sup>, Xianfeng Tang<sup>6</sup>, Qi He<sup>6</sup>, Zhigang Hua<sup>7</sup>, Bo Long<sup>7</sup>, Tong Zhao<sup>8</sup>, Neil Shah<sup>8</sup>, Amin Javari<sup>9</sup>, Yinglong Xia<sup>2</sup>, Jiliang Tang<sup>1</sup>  
<sup>1</sup>Michigan State University, <sup>2</sup>University of Oregon, <sup>3</sup>Pacific Northwest National Laboratory  
<sup>4</sup>Adobe Research, <sup>5</sup>Hippocratic AI, <sup>6</sup>Amazon, <sup>7</sup>Meta, <sup>8</sup>Snap Inc., <sup>9</sup>The Home Depot,  
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### Abstract

Retrieval-augmented generation (RAG) is a powerful technique that enhances downstream task execution by retrieving additional information, such as knowledge, skills, and tools from external sources. Graph, by its intrinsic "nodes connected by edges" nature, encodes massive heterogeneous and relational information, making it a golden resource for RAG in tremendous real-world applications. As a result, we have recently witnessed increasing attention on equipping RAG with Graph, i.e., GraphRAG. However, unlike conventional RAG, where the retriever, generator, and external data sources can be uniformly designed in the neural-embedding space, the uniqueness of graph-structured data, such as diverse-formatted and domain-specific relational knowledge, poses unique and significant challenges when designing GraphRAG for different domains. Given the broad applicability, the associated design challenges, and the recent surge in GraphRAG, a systematic and up-to-date survey of its key concepts and techniques is urgently desired. Following this motivation, we present a comprehensive and up-to-date survey on GraphRAG. Our survey first proposes a holistic GraphRAG framework by defining its key components, including query processor, retriever, organizer, generator, and data source. Furthermore, recognizing that graphs in different domains exhibit distinct relational patterns and require dedicated designs, we review GraphRAG techniques uniquely tailored to each domain. Finally, we discuss research challenges and brainstorm directions to inspire cross-disciplinary opportunities. Our survey repository is publicly maintained at <https://github.com/Graph-RAG/GraphRAG/>.

## GraphRAG



SDM25-GraphRAG

## Towards Trustworthy Retrieval Augmented Generation for Large Language Models: A Survey

Bo Ni<sup>1</sup>, Zheyuan Liu<sup>1,2</sup>, Leyao Wang<sup>1,3</sup>, Yongjia Lei<sup>3</sup>, Yuying Zhao<sup>1</sup>, Xueqi Cheng<sup>1</sup>, Qingkai Zeng<sup>2</sup>, Luna Dong<sup>4</sup>, Yinglong Xia<sup>4</sup>, Krishnamurthy Kenchadapadi<sup>5</sup>, Ryan Rossi<sup>6</sup>, Franck Dernoncourt<sup>7</sup>, Md Mehrab Tanjim<sup>8</sup>, Nesreen Ahmed<sup>9</sup>, Xiaorui Liu<sup>8</sup>, Wenqi Fan<sup>9</sup>, Erik Blasch<sup>10</sup>, Yu Wang<sup>3</sup>, Meng Jiang<sup>2</sup>, Tyler Derr<sup>1</sup>

<sup>1</sup>Vanderbilt University, <sup>2</sup>University of Notre Dame, <sup>3</sup>University of Oregon, <sup>4</sup>Meta, <sup>5</sup>Oracle Health AI, <sup>6</sup>Adobe Research, <sup>7</sup>Cisco AI Research, <sup>8</sup>North Carolina State University, <sup>9</sup>The Hong Kong Polytechnic University, <sup>10</sup>Air Force Research Lab

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{lunadong, yxia}@meta.com, {krishnamurthy.kenchadapadi}@oracle.com,  
{fryrossi, dernonco, tanjim}@adobe.com, {nesahmed@cisco.com, xliu96@ncsu.edu, wenqi.fan@polyu.edu.hk, erik.blasch.1@us.af.mil

### Abstract

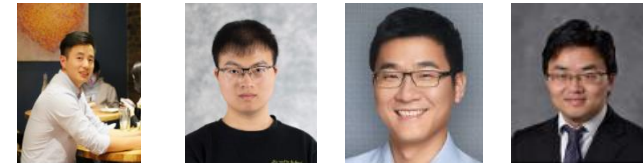
Retrieval-Augmented Generation (RAG) is an advanced technique designed to address the challenges of Artificial Intelligence-Generated Content (AIGC). By integrating context retrieval into content generation, RAG provides reliable and up-to-date external knowledge, reduces hallucinations, and ensures relevant context across a wide range of tasks. However, despite RAG's success and potential, recent studies have shown that the RAG paradigm also introduces new risks, including robustness issues, privacy concerns, adversarial attacks, and accountability issues. Addressing these risks is critical for future applications of RAG systems, as they directly impact their trustworthiness. Although various methods have been developed to improve the trustworthiness of RAG methods, there is a lack of a unified perspective and framework for research in this topic. Thus, in this paper, we aim to address this gap by providing a comprehensive roadmap for developing trustworthy RAG systems. We place our discussion around five key perspectives: reliability, privacy, safety, fairness, explainability, and accountability. For each perspective, we present a general framework and taxonomy, offering a structured approach to understanding the current challenges, evaluating existing solutions, and identifying promising future research directions. To encourage broader adoption and innovation, we also highlight the downstream applications where trustworthy RAG systems have a significant impact. For more information about the survey, please check our GitHub repository<sup>\*</sup>.

## Trustworthy RAG



We really appreciate the travel support from SIAM for some of our teammates in presenting this tutorial!

## Lead Tutors



## Survey Collaborators (Order by Random)

