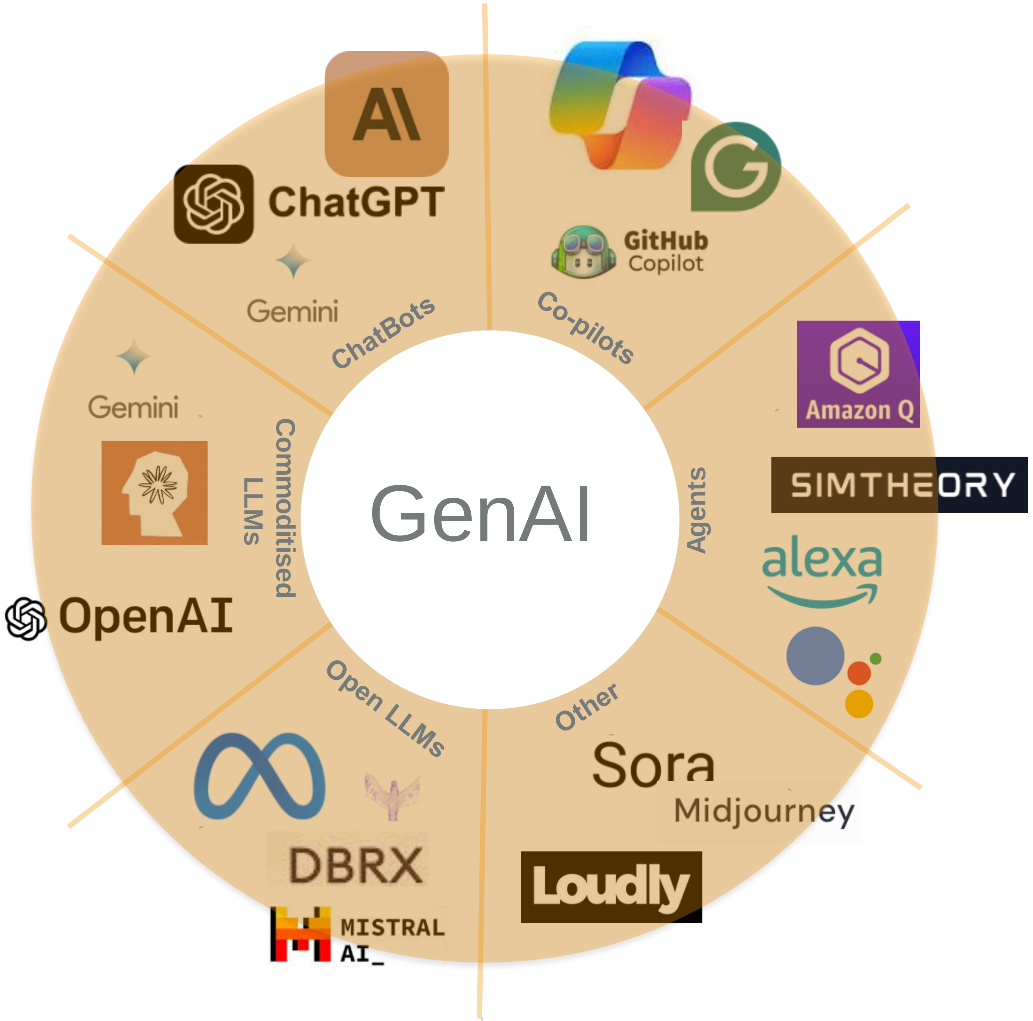
Pistoia Alliance 2024 London conference

Ontologies and LLMs: *Democratising Scientific Data*

Joe Mullen, PhD

24th April 2024

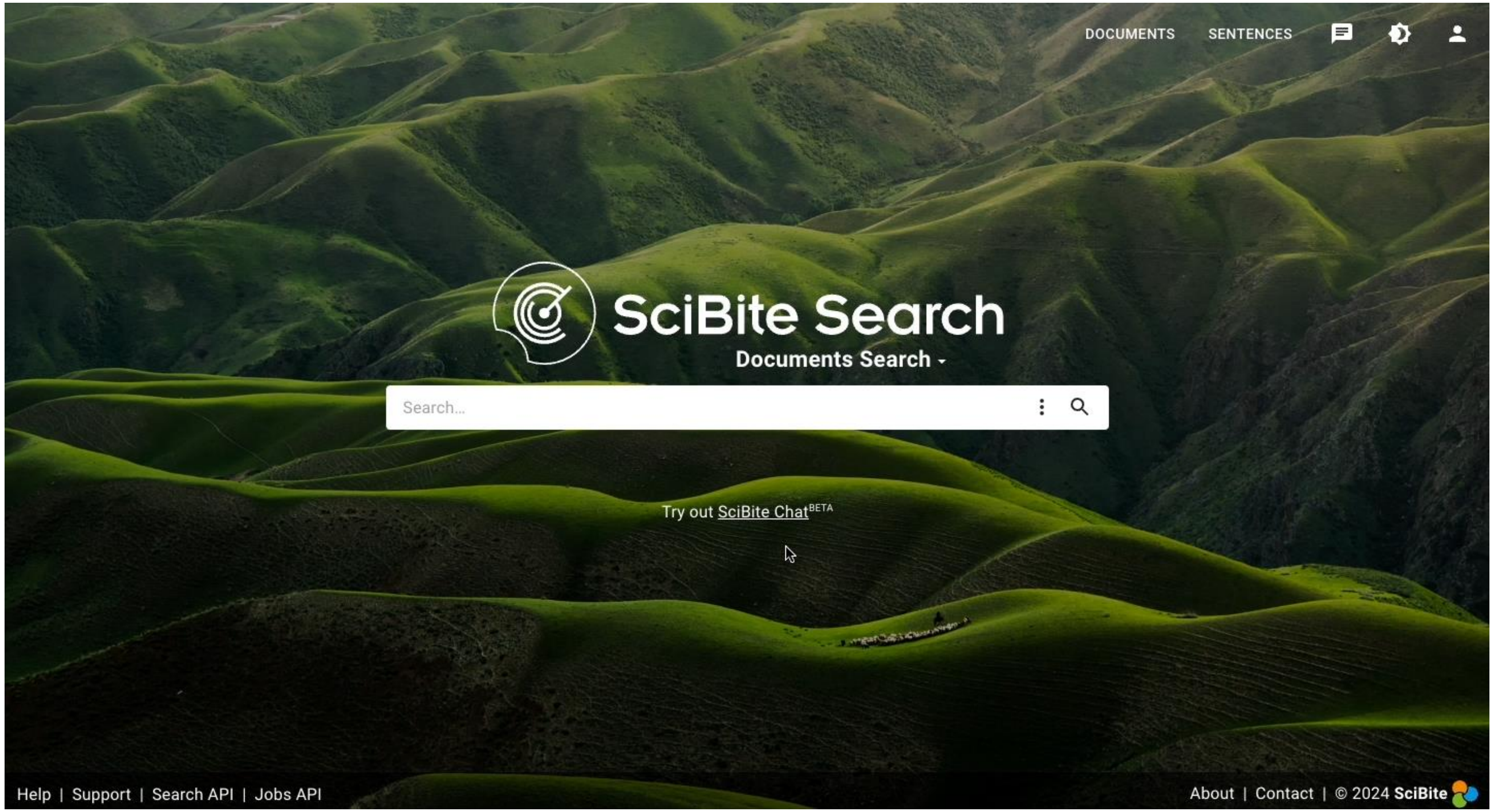

GenAI
ChatBots
ChatGPT
Gemini
Co-pilots
GitHub Copilot
Agents
Amazon Q
SIMTHEORY
alexa
Other
Sora
Midjourney
Loudly
Open LLMs
DBRX
MISTRAL AI_
Commoditised LLMs
Gemini
OpenAI

Roll out and adoption of GenAI brings changes to **user expectations** when interfacing with technology

How can GenAI enable insight within life sciences?

SciBite Chat

Launched April '24!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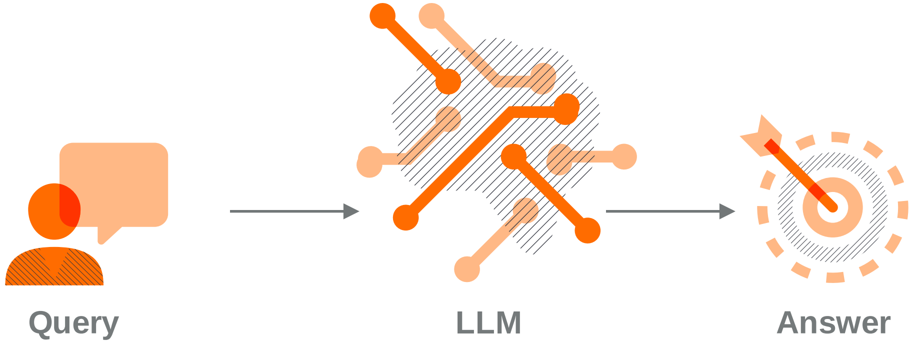
Democratising data; speeding up insight

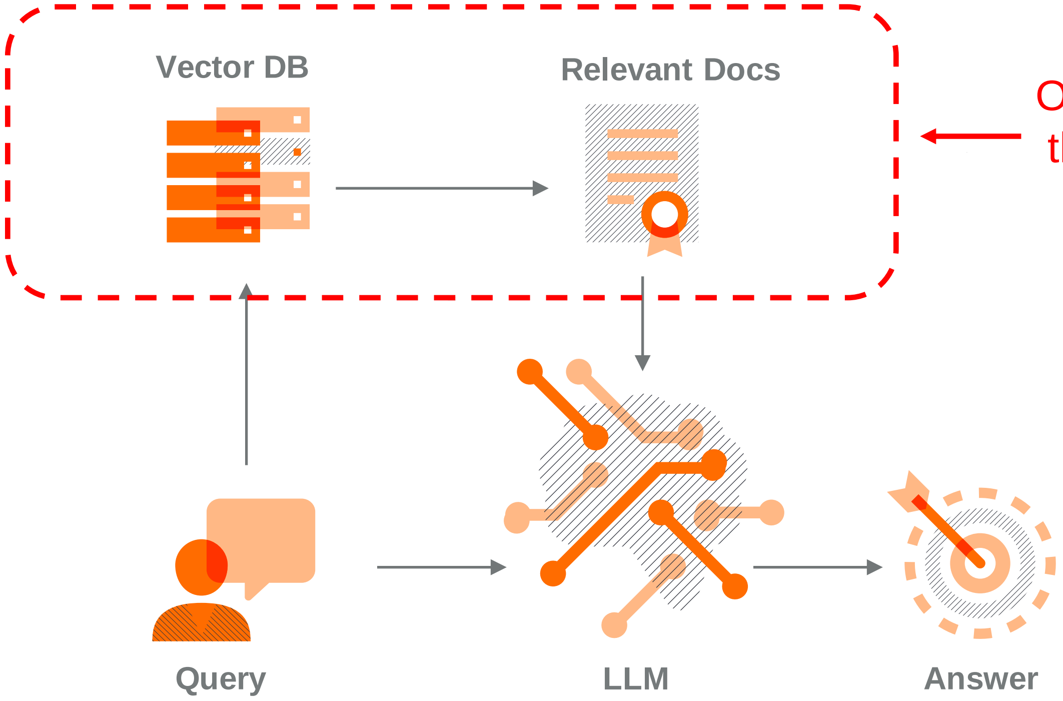
But how did we get here?


Query
LLM
Answer

Did we just ask an LLM direct?

accuracy ✗ | transparency ✗ | flexibility ✗

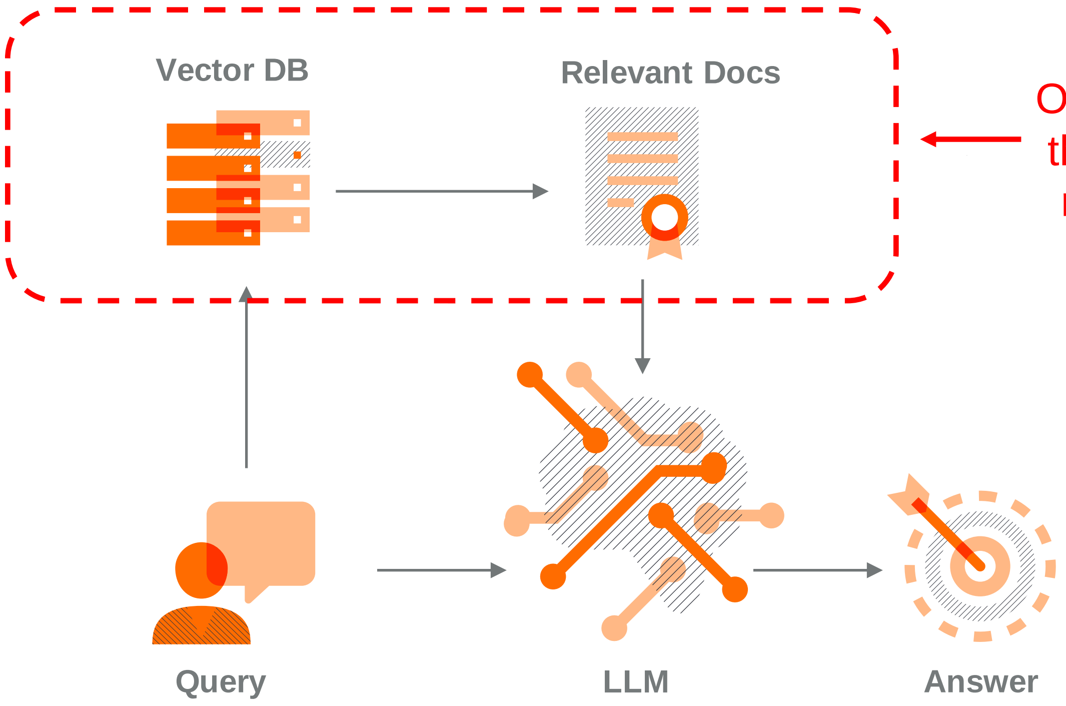
Not quite....


Vector DB
Relevant Docs
Query
LLM
Answer

Only as good as the information retrieval step!

RAG architecture

*Retrieval Augmented Generation


Vector DB
Relevant Docs
Query
LLM
Answer

Only as good as the information retrieval step!

Did we make use of a RAG architecture with **vector-based** information retrieval?

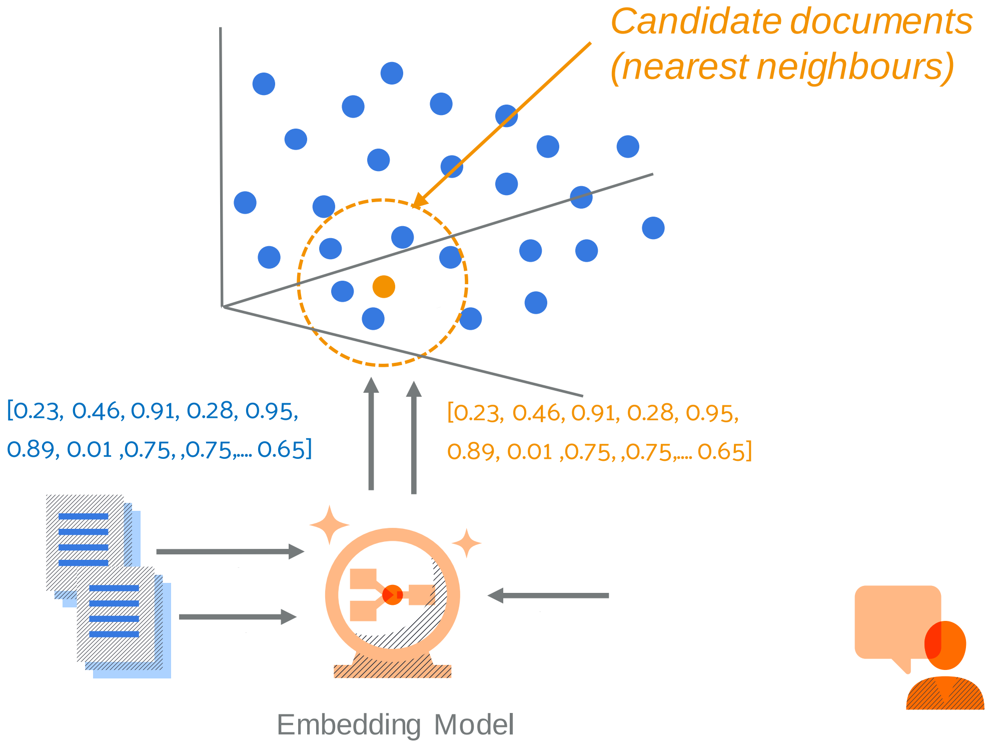
accuracy	transparency	flexibility
?	✗	✓

Not quite....

*Retrieval Augmented Generation

transparency **human explainability**

*Vector-based retrieval – **what** is related, not **how***



Candidate documents (nearest neighbours)

[0.23, 0.46, 0.91, 0.28, 0.95, 0.89, 0.01 ,0.75, ,0.75,.... 0.65]

[0.23, 0.46, 0.91, 0.28, 0.95, 0.89, 0.01 ,0.75, ,0.75,.... 0.65]

Embedding Model

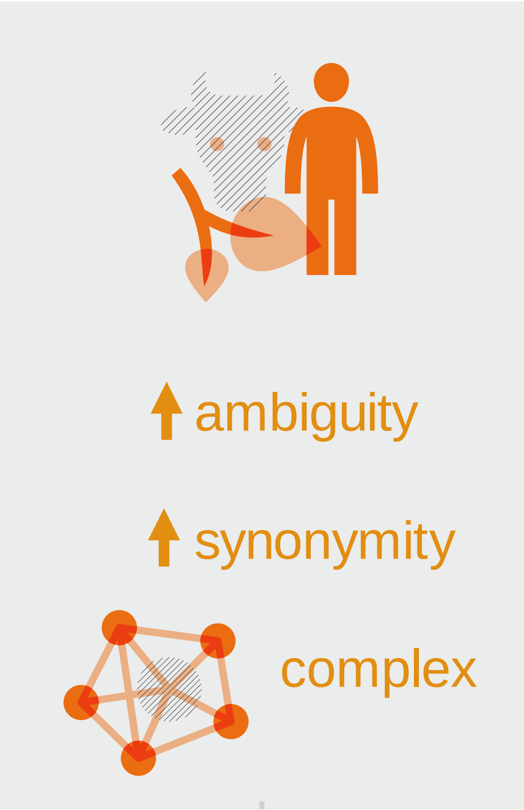
Amazing technology, almost like magic.... **but** how do you explain magic?

There is another way...

Building on domain knowledge

We’ve spent **a long** time organising the chaos in data....

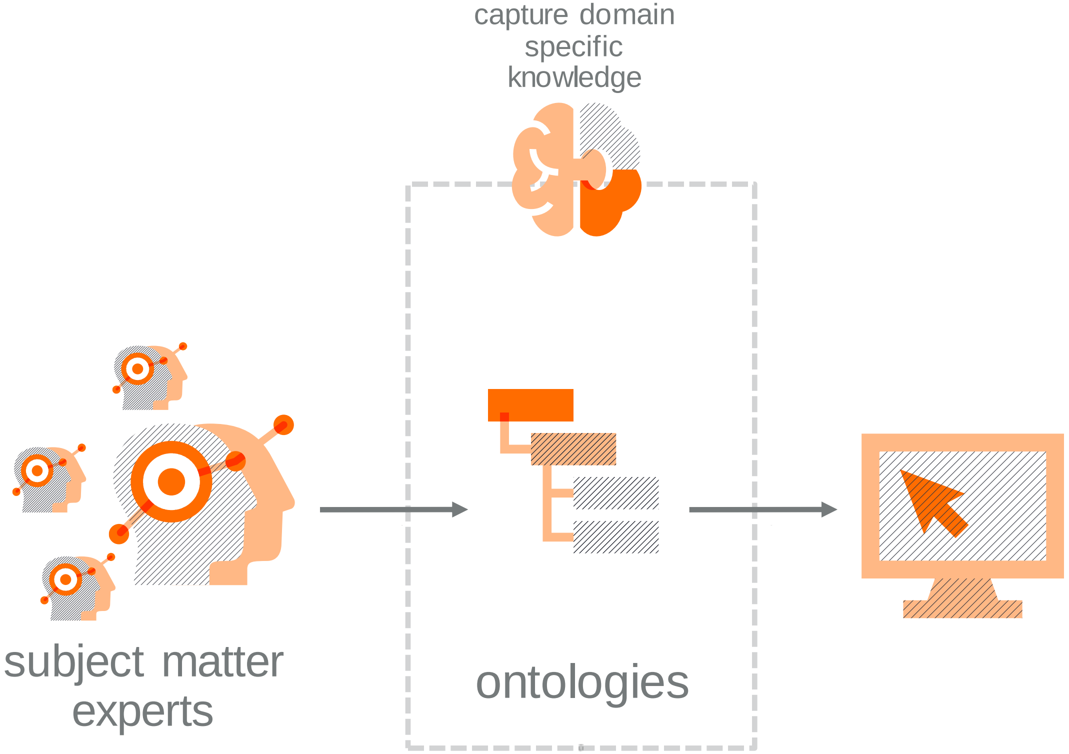
Life Sciences



↑ ambiguity

↑ synonymity

complex



capture domain specific knowledge

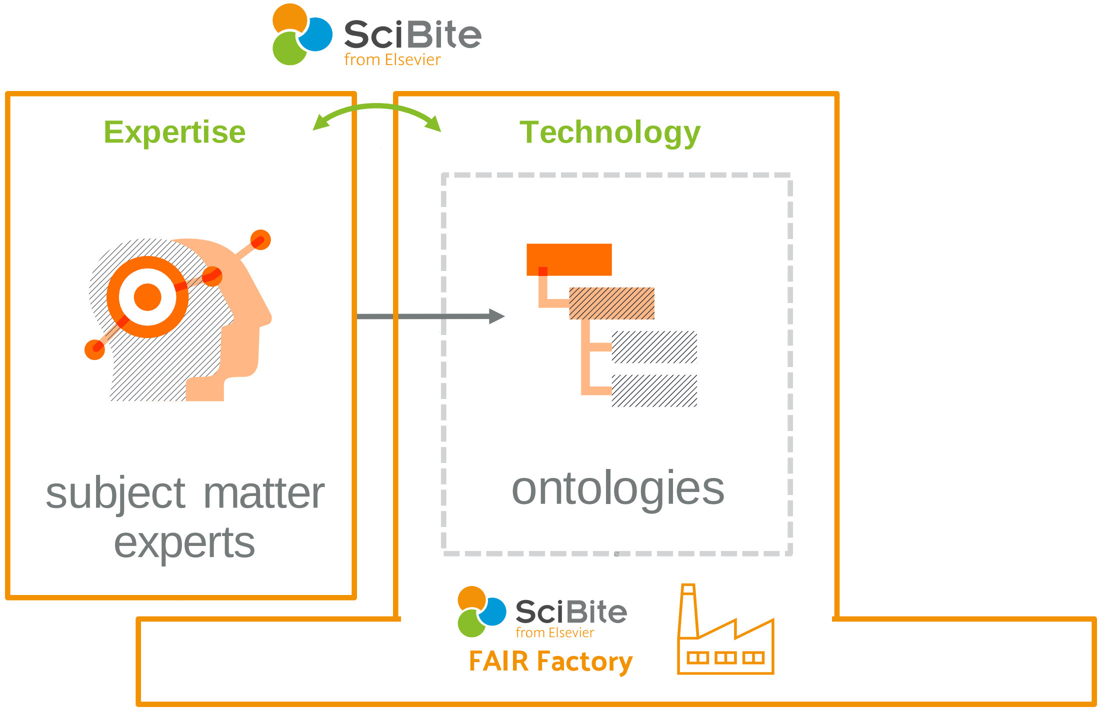
subject matter experts

ontologies

internal
external
collaborative

Building on domain knowledge

We've spent a **long** time organising the chaos in data....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Expertise
Technology
subject matter experts
ontologies
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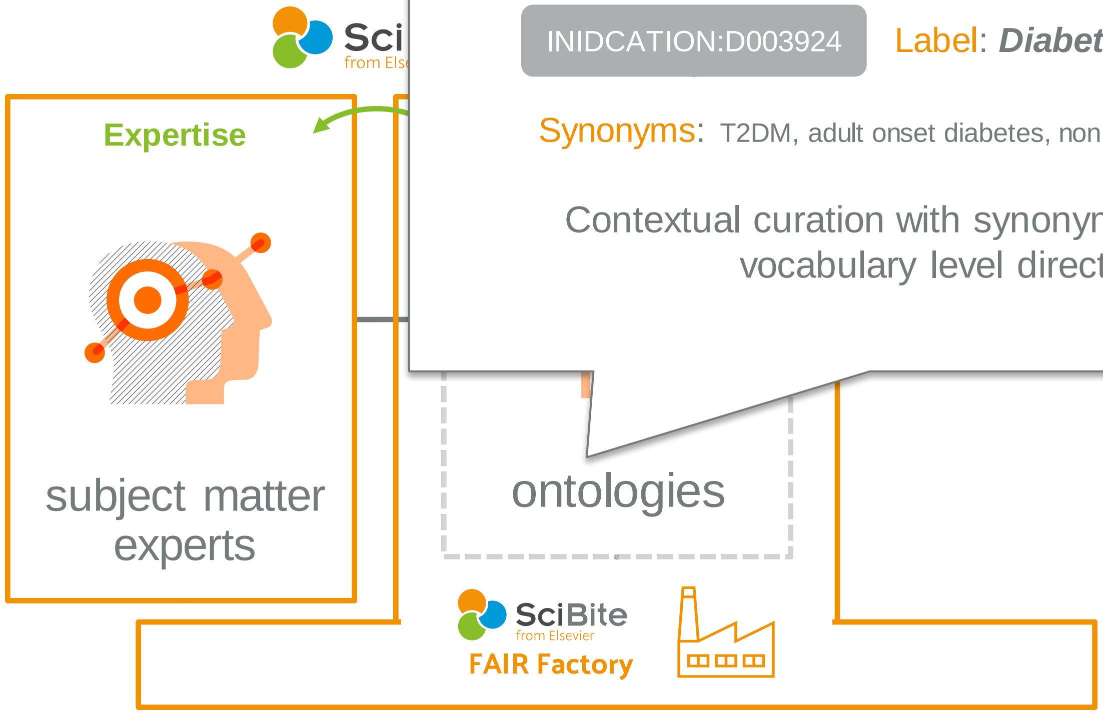
FAIR Factory

Building on domain knowledge

We’ve spent a **long** time organising the chaos i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from Else
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transforming ontologies for named entity recognition

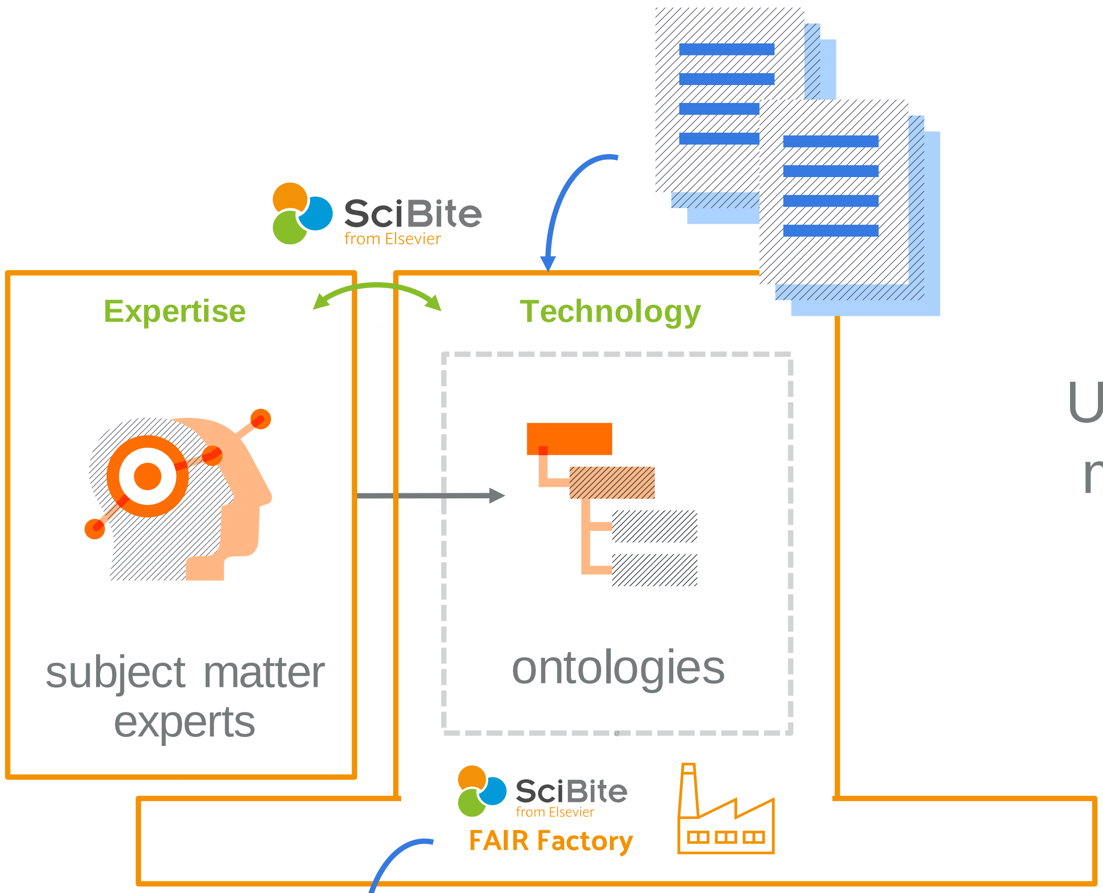
INIDCATION:D003924 Label: ***Diabetes Mellitus, Type 2***

Synonyms: T2DM, adult onset diabetes, non insulin-dependent DM

Contextual curation with synonym switches and vocabulary level directives

Building on domain knowledge

We've spent a **long** time organising the chaos in data....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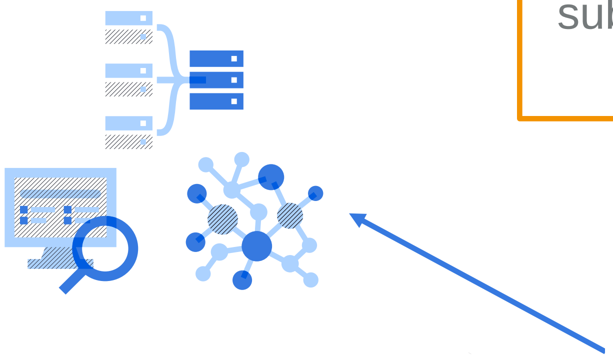
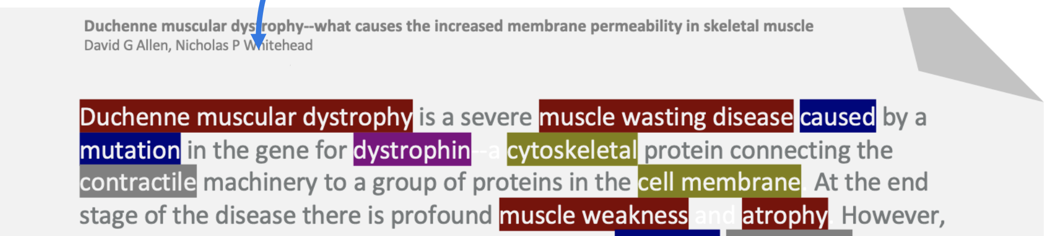
Unstructured text to machine readable, semantic data



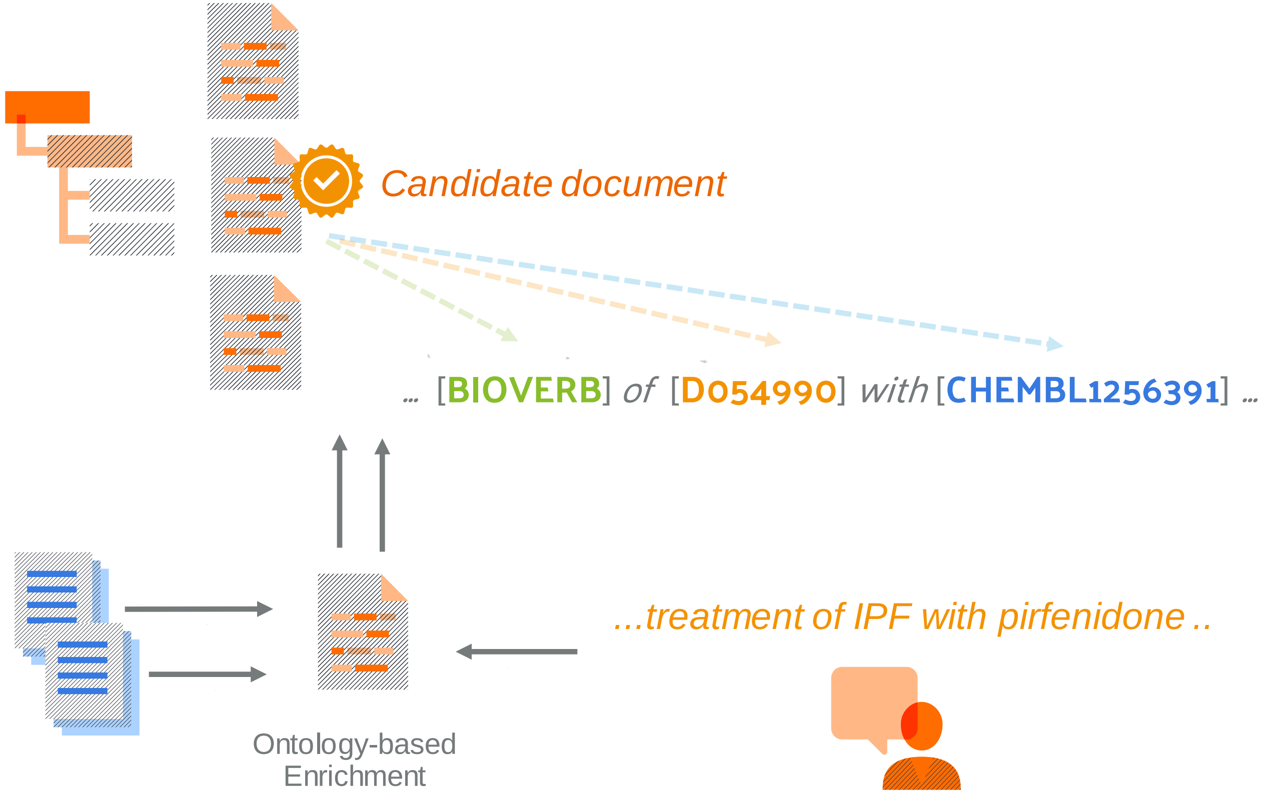


Duchenne muscular dystrophy--what causes the increased membrane permeability in skeletal muscle
David G Allen, Nicholas P Whitehead

Duchenne muscular dystrophy is a severe muscle wasting disease caused by a mutation in the gene for dystrophin--a cytoskeletal protein connecting the contractile machinery to a group of proteins in the cell membrane. At the end stage of the disease there is profound muscle weakness and atrophy. However,

transparency **human explainability**

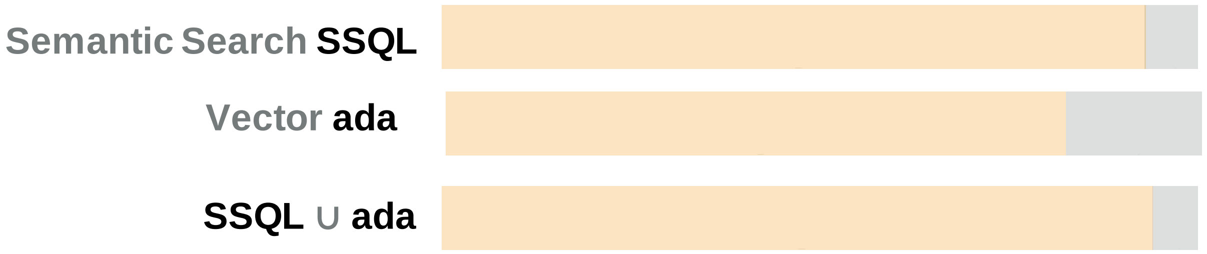
*ontology-based retrieval – what it **is**, **what** is related, **and** how*


Candidate document
… [BIOVERB] of [D054990] with [CHEMBL1256391] …
…treatment of IPF with pirfenidone ..
Ontology-based Enrichment

Looking at the accuracy of the information retrieval approaches

Information Retrieval

Reviewing accuracy, internal benchmark



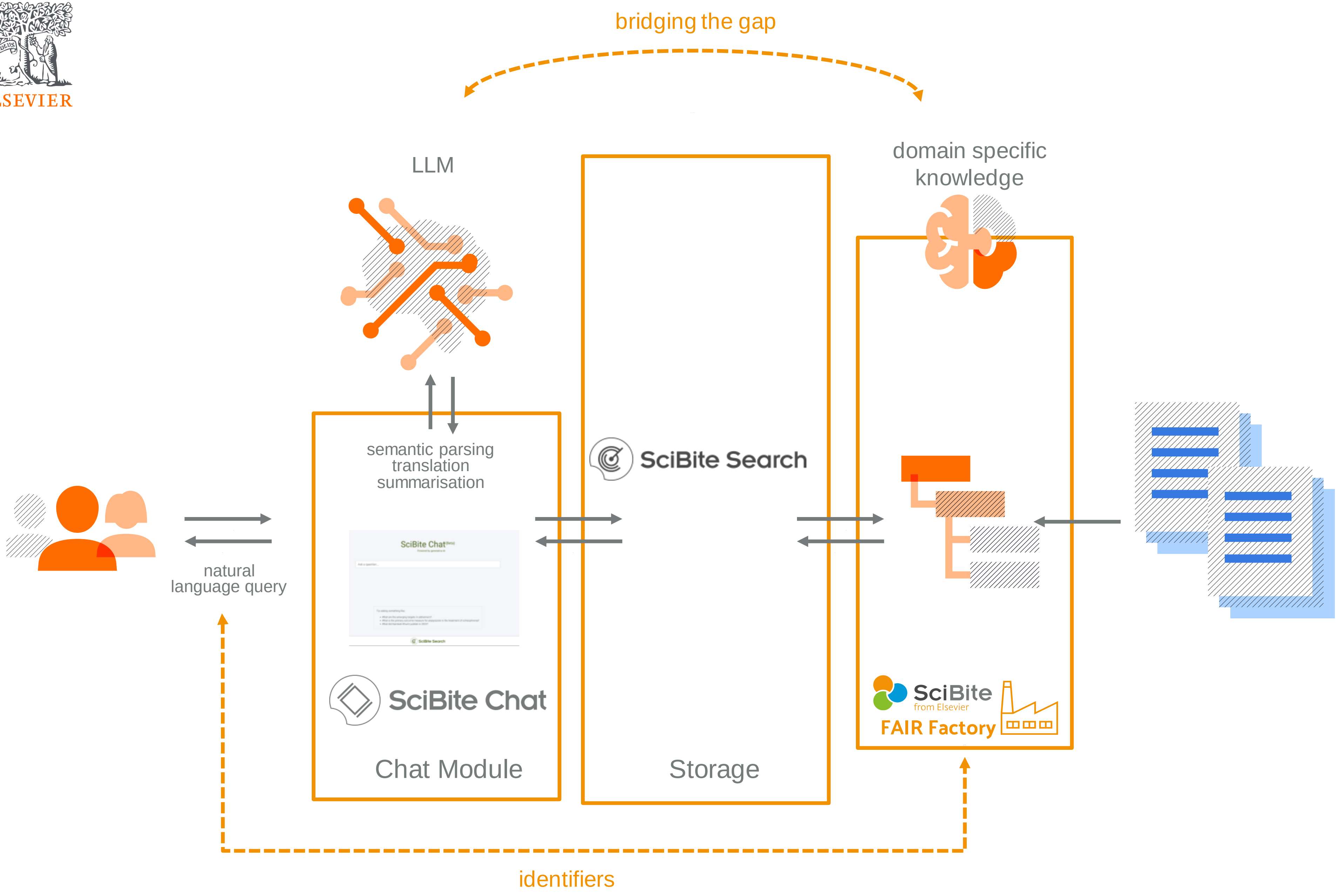
Questions with at least one answer match

We used a RAG architecture with SciBite ontology-based information retrieval....

ELSEVIER

Let’s take a closer look at

SciBite Chat



bridging the gap

LLM

domain specific
knowledge

semantic parsing
translation
summarisation

SciBite Chat

SciBite Search

natural
language query

SciBite Chat

Chat Module

Storage

SciBite
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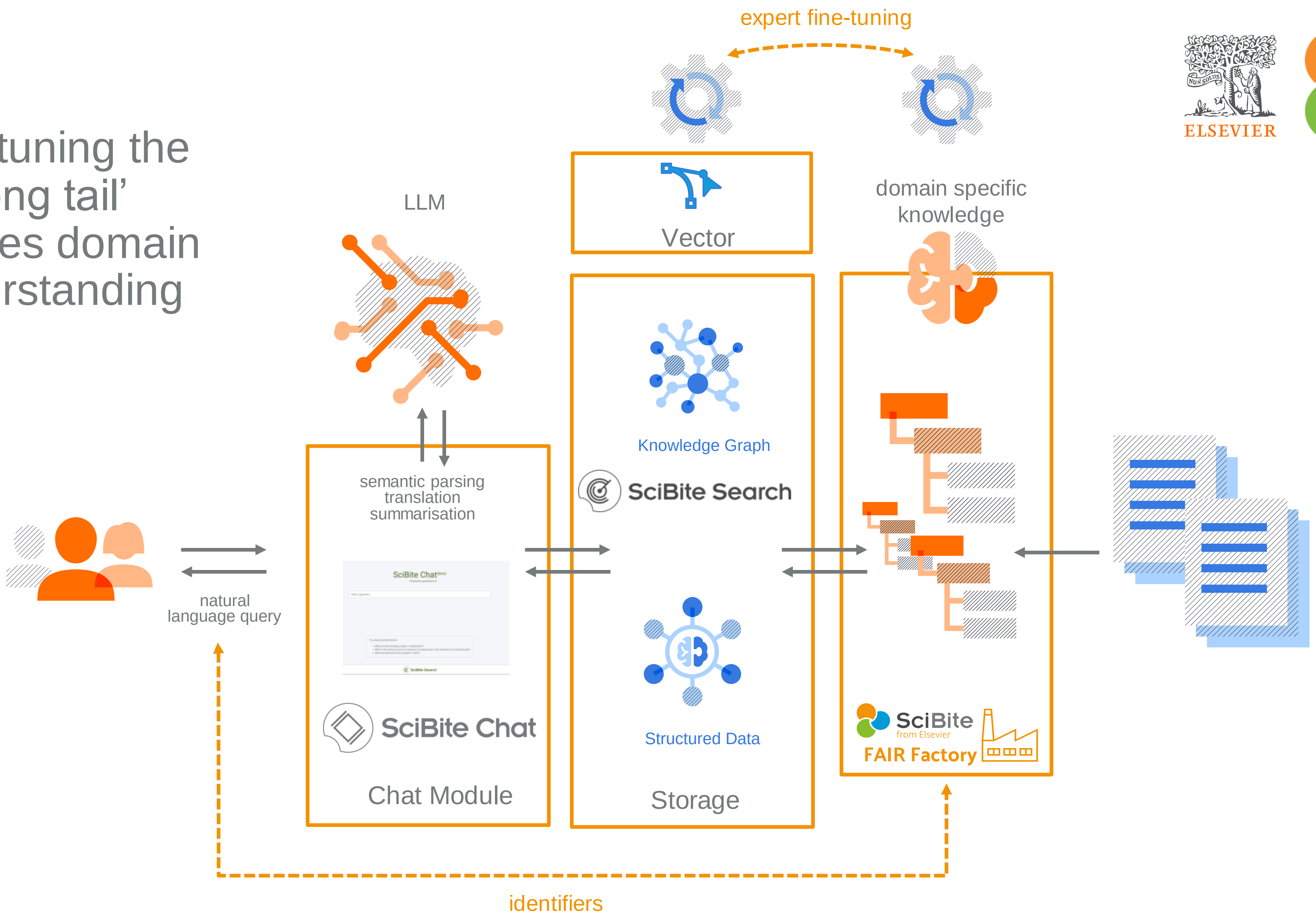
identifiers

Flexibility
Deployment
Security
Data
Ontologies

The vision

Fine-tuning the ‘long tail’ requires domain understanding


expert fine-tuning
LLM
Vector
domain specific knowledge
semantic parsing
translation
summarisation
SciBite Chat
Chat Module
natural language query
Knowledge Graph
SciBite Search
Structured Data
Storage
SciBite from Elsevier
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identifiers

TL;DR

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Data

Expertise

Technology

- accuracy
- transparency
- flexibility
- user expectations

We speak your language – hear what your data has to say!

SciBite Chat

Acknowledgements

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Divya Nair

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Thanks for listening!

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Take the next step
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Come and talk to the team!

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