Before we start ...

LLM systems need a different way of thinking

Where traditional AI is *good* for processing data and predicting future data states, ... LLM systems are *good* for extracting relevance and reasoning from information.
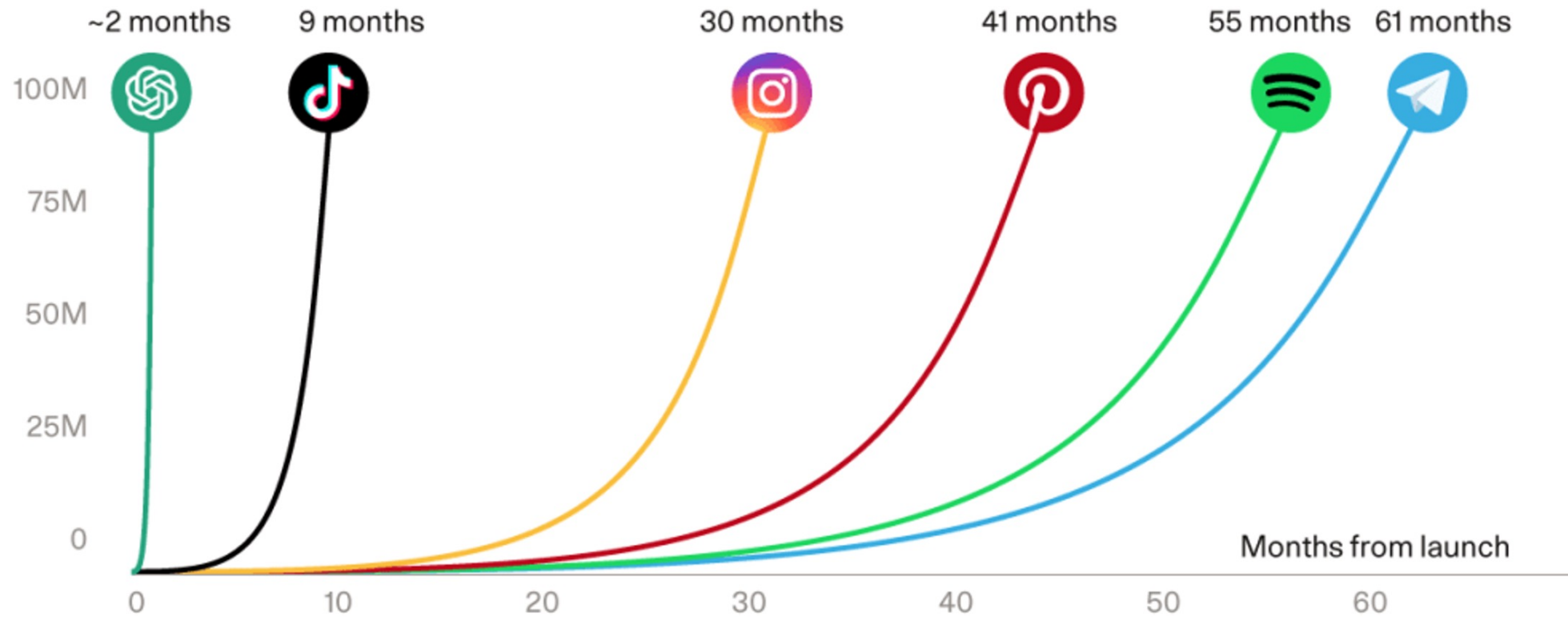
LLM systems are like new grad hires:
- they are eager to say something to help,
- often not sure if they understand your question, and
- are happy to deep dive where you tell them, but many times miss the context.

This just gets harder when dealing in science!

Path to 100 Million Users

Forbes

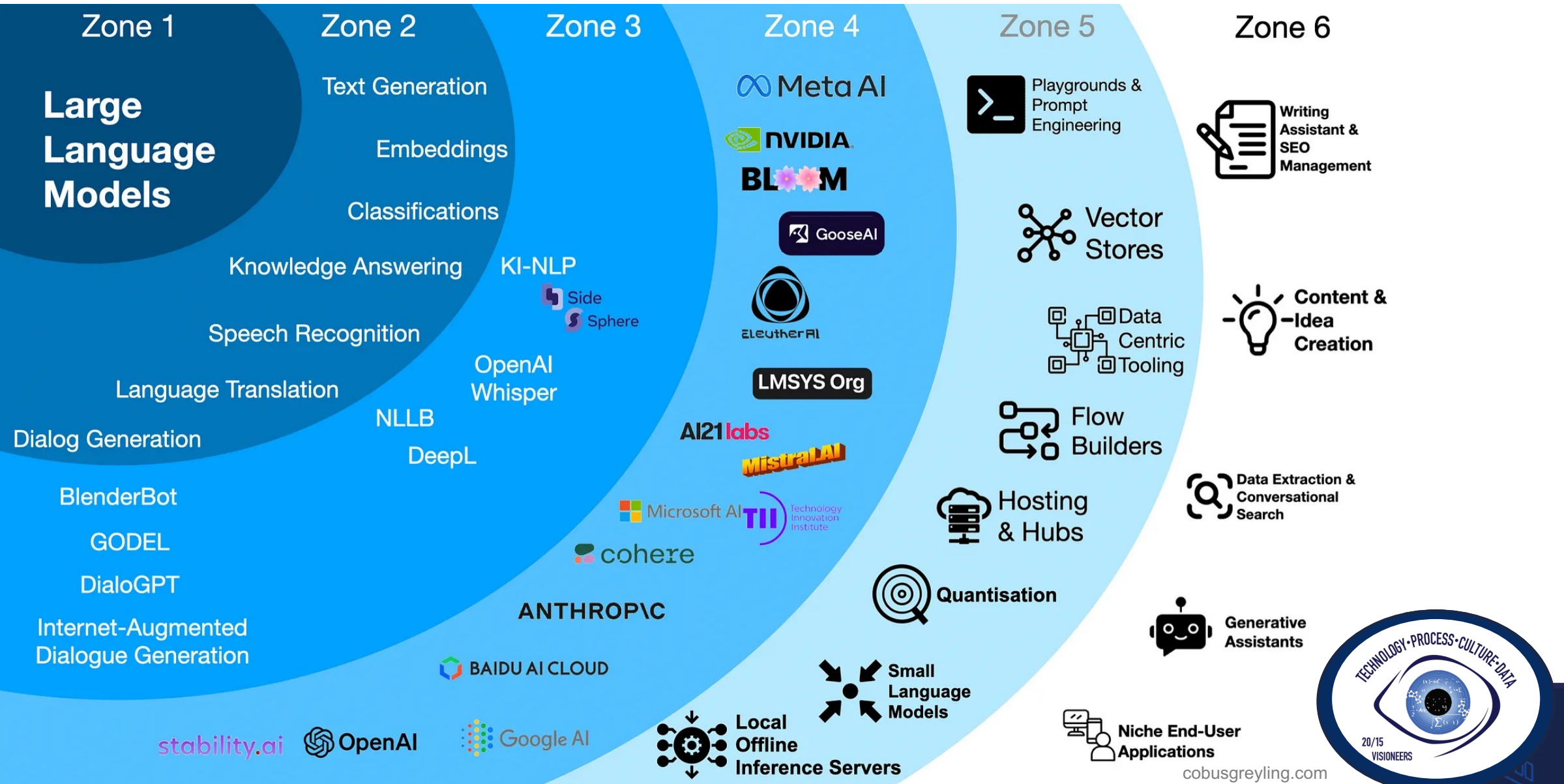# Agentic AI: The Next Big Breakthrough That's Transforming Business And Technology

Think of agentic AI as a digital assistant on steroids.

Instead of just answering your questions or performing simple tasks, it can take initiative, solve complex problems, and adapt its approach based on changing circumstances.

It's like having a tireless, hyper-intelligent intern who not only follows your instructions but also anticipates your needs and comes up with creative solutions you might never have considered.
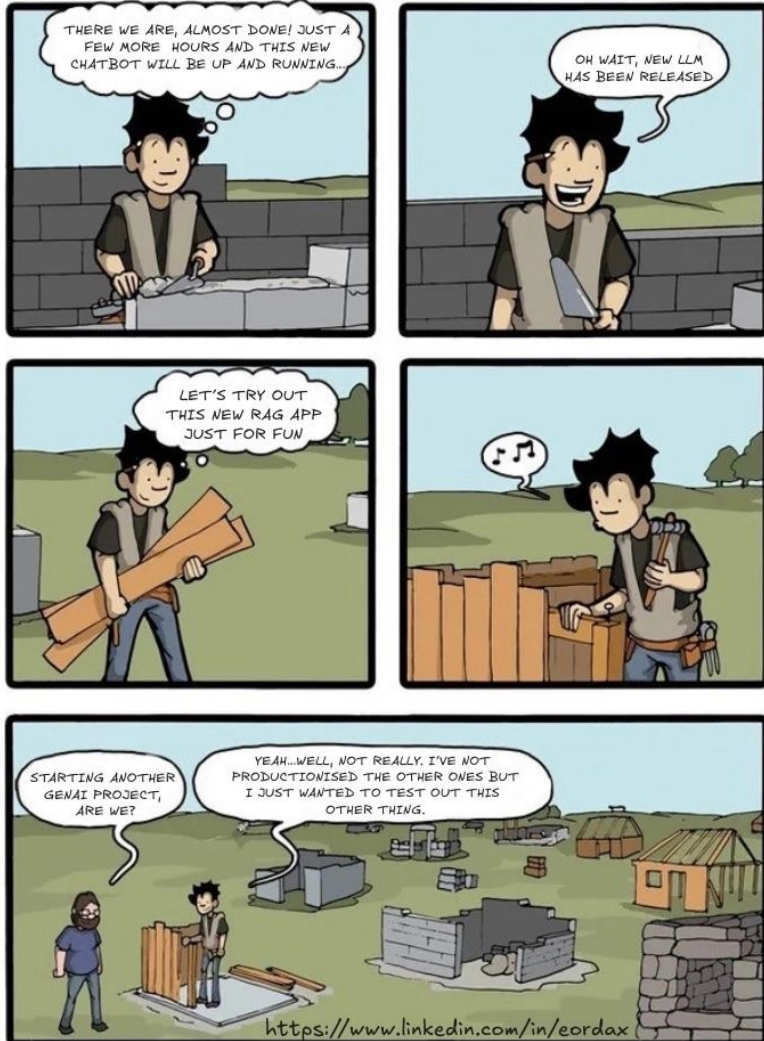
The LLM ecosystem is complex and evolving fast

Zone 1 — Large Language Models

Zone 2
- Text Generation
- Embeddings
- Classifications
- Knowledge Answering
- Speech Recognition
- Language Translation
- Dialog Generation
- BlenderBot
- GODEL
- DialoGPT
- Internet-Augmented Dialogue Generation

Zone 3
- KI-NLP
- Side Sphere
- OpenAI Whisper
- NLLB
- DeepL
- Microsoft AI
- TII Technology Innovation Institute
- cohere
- ANTHROP\C
- BAIDU AI CLOUD

Zone 4
- Meta AI
- NVIDIA
- BLOOM
- GooseAI
- EleutherAI
- LMSYS Org
- AI21 labs
- MistralAI
- Local Offline Inference Servers
- Small Language Models

Zone 5
- Playgrounds & Prompt Engineering
- Vector Stores
- Data Centric Tooling
- Flow Builders
- Hosting & Hubs
- Quantisation

Zone 6
- Writing Assistant & SEO Management
- Content & Idea Creation
- Data Extraction & Conversational Search
- Generative Assistants
- Niche End-User Applications

stability.ai   OpenAI   Google AI

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5

Operational and Business Considerations

Technical debt: It often costs more to integrate and manage new technology than develop it. LLM systems are easy to plug in, but difficult to monitor and upgrade.

Reliability: LLM systems work "some to most of the time". They are inherently guessing what to do next, which creates variability in their answers., impacting reproducibility also.

API/token costs: LLM systems may offer much promise, but the LLM providers make significant money every month if token requests are not managed carefully. Submitting long prompts and publications to LLMs could use a lot of tokens!

Adaptability to new technologies: This year it is all about agentic systems, next year it will be something else. And the models themselves are advancing rapidly, making the balance between systems design and LLM choice very dynamic. P.S. Many of the advancements seem big but are incremental.

6

Technical Considerations

Lack of true reasoning and understanding:
Agentic AI systems and LLMs in general rely on probability-driven outputs rather than genuine comprehension or reasoning.

Potential for hallucinations and incorrect outputs:
LLMs are prone to generating "hallucinations," where the model produces information that appears factual but is inaccurate. In an agentic system, this can lead to incorrect autonomous decisions and actions.

Challenges with transparency and accountability:
Agentic AI systems often operate as black boxes, making it difficult to trace the rationale behind their decisions. Chain-of-Thought behavior is improving this.

Biases in decision-making:
Since LLMs are trained on large datasets (mainly) from the internet, they may inherit biases present in the data. They may also inherit biases when leveraging publications (RAG databases).

PythiaAI™
Research Assistant

Enabling Rapid Discovery

Client Workflow — Scientists — PythiaAI™
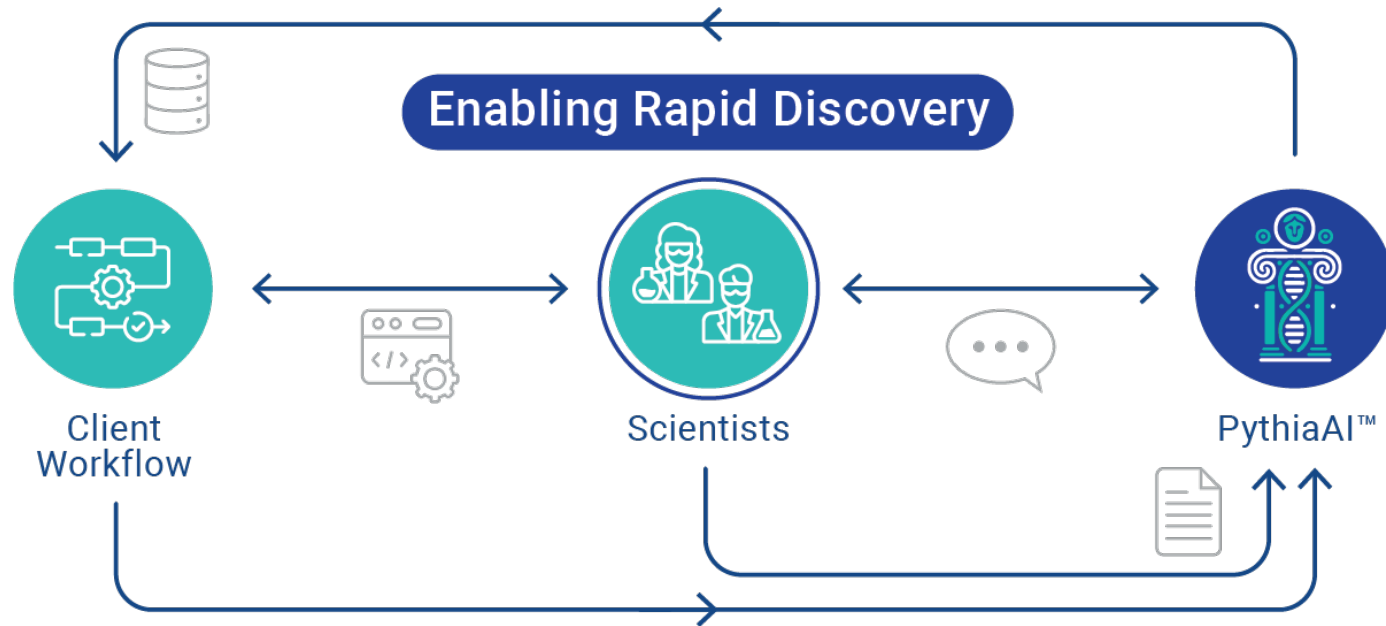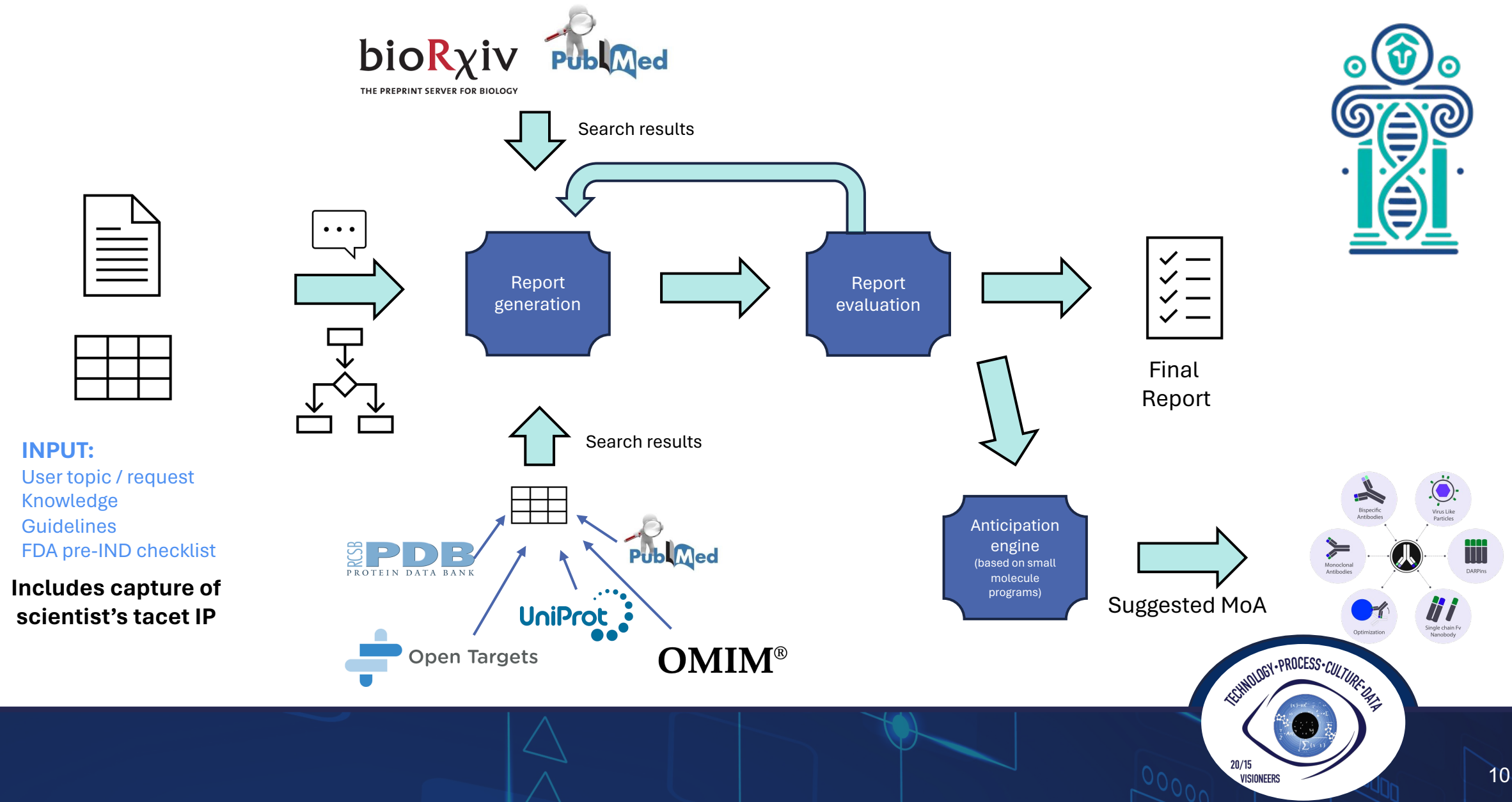
- Plug'n'play design and remote management reduce technical debt

- Simple modular architecture, enabling new technologies to be swapped in

- Works across diverse use-cases, from drug discovery to lab operations to medical research

- Optimized to minimize API / token costs

- Tuned & tested to client use case to ensure reliability

- Includes scoring for Novelty, Relevance, and Hallucination

- Applicable to a diverse range of scientific workflows in life sciences and beyond

Implementation Approach for Antibody Drug Discovery

INPUT:
User topic / request
Knowledge
Guidelines
FDA pre-IND checklist

Includes capture of scientist's tacet IP

Search results

Report generation

Report evaluation

Final Report

Search results

Anticipation engine (based on small molecule programs)

Suggested MoA

Data Curation

STEPS

- Map search results from Uniprot & PubMed

- Rank structures in the combined list based on PDB and mutation type

- Identify relevant disease targets and therapies

Pubmed:132K ; UniProt: 14K

Verified structures: 1,082

Identifying Wild-Type/Mutation

Ranking
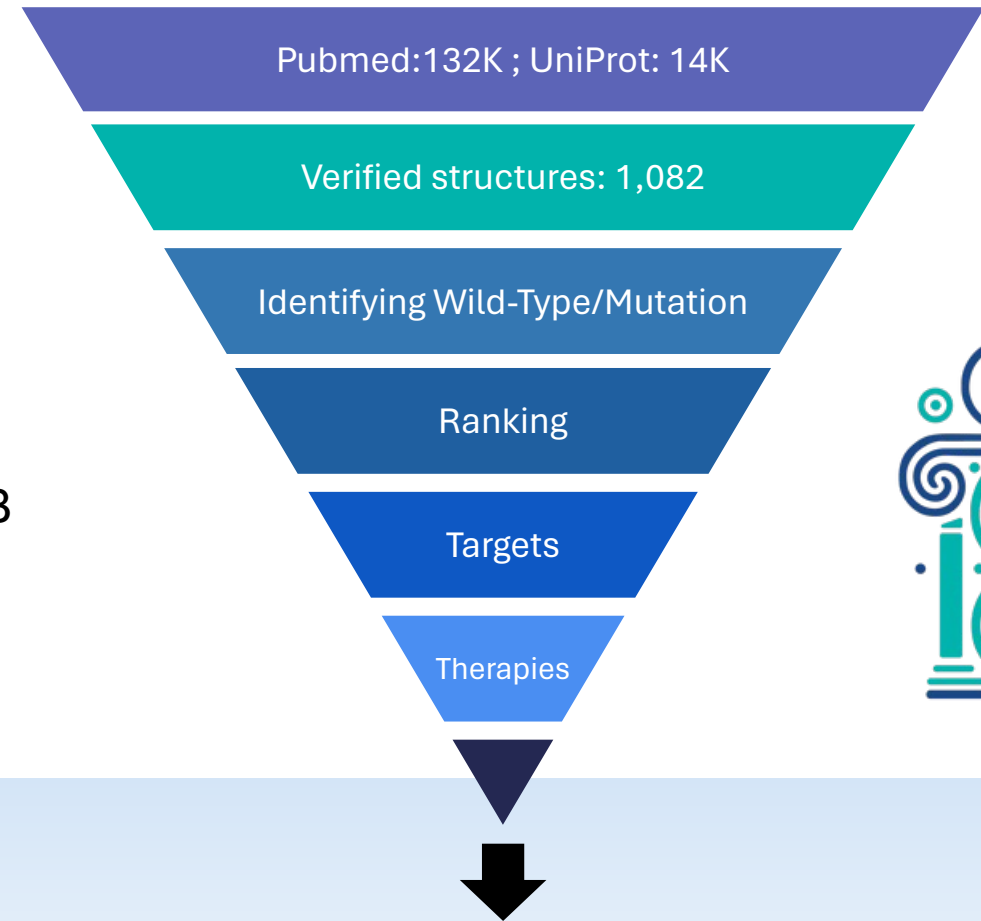
Targets

Therapies

RESULTS for "Antibody design in EGFR"

UniProt ID	Protein Na	Gene Nam	Organism	PDB ID	Resolution	Mutated Type	Disease Target	Known Therapies	PubMed ID	Title	Journal	Authors
Q99527	G-protein (	GPER1	Homo sapi	8XOF	2.6	Wild-Type	Breast cancer	No	38744981	Structural	Cell Res.	Liu, H., Guo, S., Dai, A., Xu, P., Li, X., Huang, S., He, X., Wu, K., Zhang, X., Yang, D., Xie, X., Xu, H.E.
P01133	Pro-epider	EGF	Homo sapi	1NQL	2.8	Wild-Type	Neurodegenrative	No	12620237	EGF activa	Mol.Cell	Ferguson, K.M., Berger, M.B., Mendrola, J.M., Cho, H., Leahy, D.J., Lemmon, M.A.
P00533	Epidermal	EGFR	Homo sapi	8A27	1.07	Wild-Type	Lung Cancer	Inhibitor inhibitor	36178776	Discovery (	J.Med.Che	Obst-Sander, U., Ricci, A., Kuhn, B., Friess, T., Koldewey, P., Kuglstatter, A., Hewings, D., Goergler, A.,
A8IP97	receptor pi	Egfr	Rattus non	1I31	2.5	Wild-Type	N/A	N/A	N/A	MU2 ADAP	To be Publi	Modis, Y., Boll, W., Rapoport, I., Kirchhausen, T.
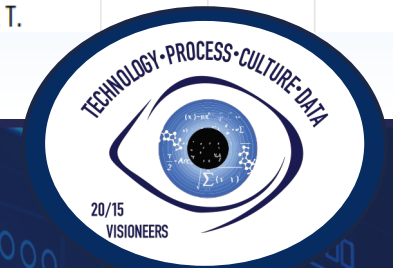
Customer Success Story

Quine Biologics, Inc.
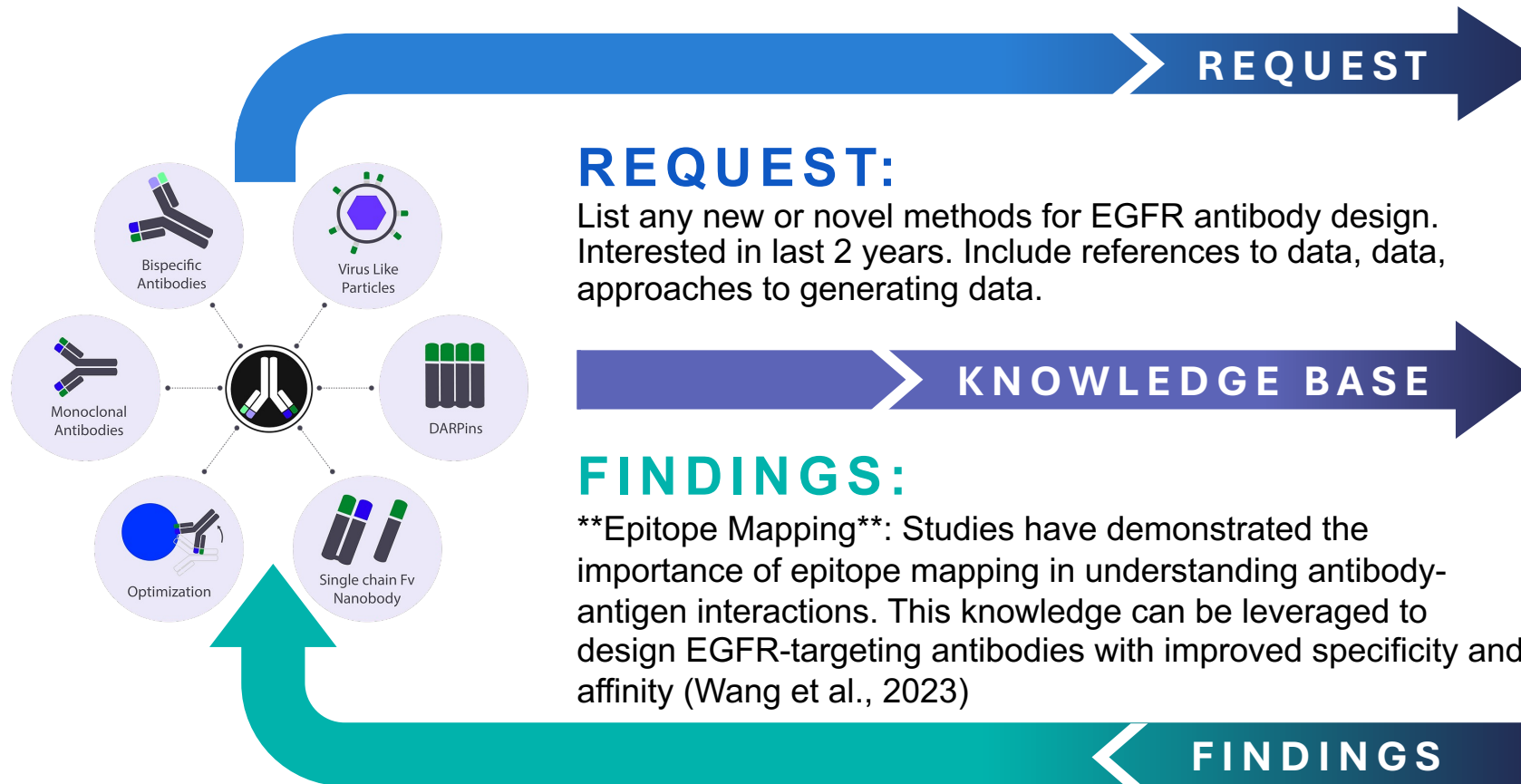
REQUEST

REQUEST:

List any new or novel methods for EGFR antibody design. Interested in last 2 years. Include references to data, data, approaches to generating data.

KNOWLEDGE BASE

FINDINGS:

Epitope Mapping: Studies have demonstrated the importance of epitope mapping in understanding antibody-antigen interactions. This knowledge can be leveraged to design EGFR-targeting antibodies with improved specificity and affinity (Wang et al., 2023)

FINDINGS

PythiaAI™

Your Research Assistant

Welcome to the Drug Discovery version of PythiaAI.

Please contact us to access the Lab Operations and Medical Research versions.

Enter your scientific topic of interest:

List any new or novel methods for EGFR antibody design. Interested in last 2 years. Include references to data, data, approaches to generating data.

Submit

Quine Biologics' Knowledgebase has been read in.

PubMed search results saved to ./output/Search_results_PubMed_20240908-162757.txt

Summary for PubMed saved to ./output/Summary_PubMed_20240908-162814.pdf

BioRxiv search results saved to ./output/Search_results_bioRxiv_20240908-162816.txt

Summary for bioRxiv saved to ./output/Summary_bioRxiv_20240908-162924.pdf

PythiaAI run complete.

Please check your Output directory for the Summary PubMed & bioRxiv reports and search results.

Bispecific Antibodies

Virus Like Particles

Monoclonal Antibodies

DARPins

Optimization

Single chain Fv Nanobody

Press Release

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Quine Biologics, Inc.

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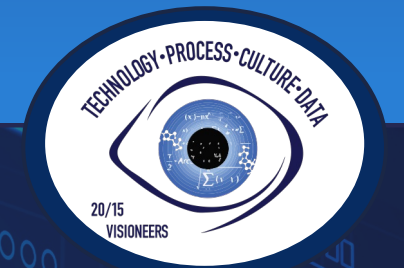
For more info about this partnership:
http://20visioneers15.com/pythiaai

"StableBody Technologies has built a leading-edge computational system for linear sequence of predicting enhanced stability and affinity in proteins.

With PythiaAI™, we are now able to rapidly discover new hypotheses for protein stability, both in our experiments and in literature.

This addition has immediately solved the problem of searching the universe for new optimized proteins."

- Harry Horn, CEO StableBody Technologies

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THANK YOU

What would you like to see PythiaAI™ do?

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