

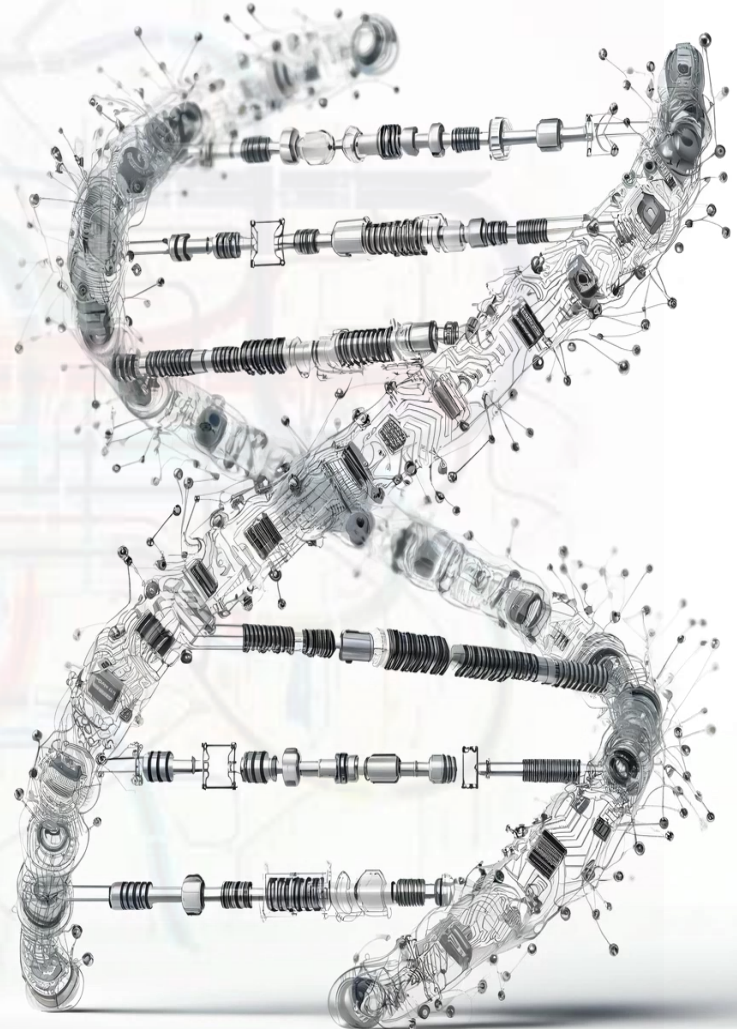


# A practical guide to AI tools for life scientists.

Peering into the Future of  
AI-Augmented Scientific Research.



Michael Kuiper  
8<sup>th</sup> May 2024.



# Overview:

## What:

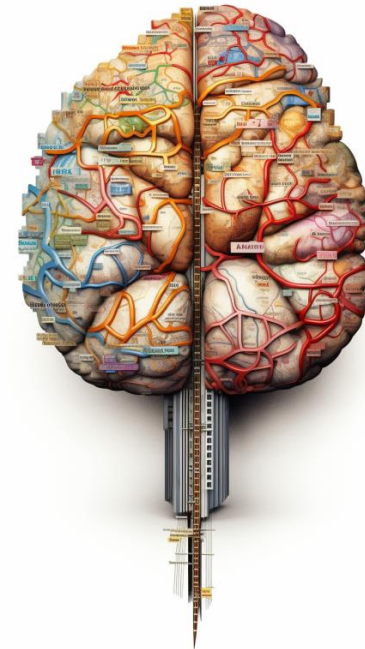
- The recent timeline of Large Language Models.
- What are LLMs anyway?

## Why:

- Why use LLMS over search engines?
- The information challenge.

## How:

- LLM based Agents, Assistants and Tools.
- How we might use AI for research & dev. (demos)
- How to get the most from your 'cognitive co-pilot' and how to avoid the pitfalls.



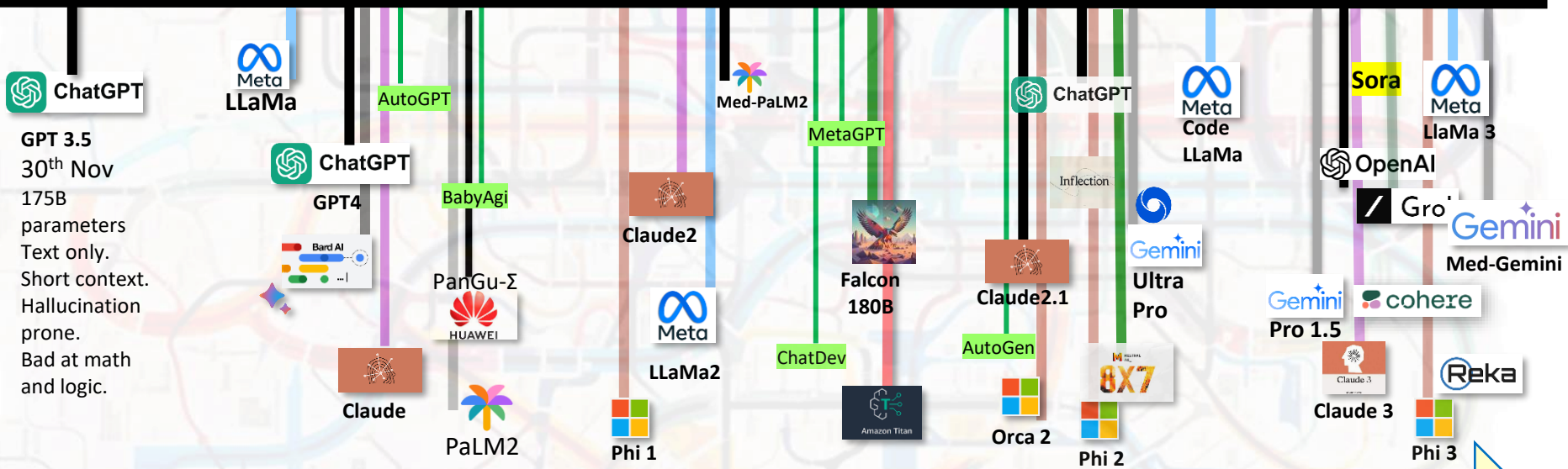
# The Rise of Large Language Models.

2022

2023

2024

Nov Dec Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec Jan Feb Mar Apr May



Multimodal abilities  
+ Increasing context length



# What are LLMs anyway?:

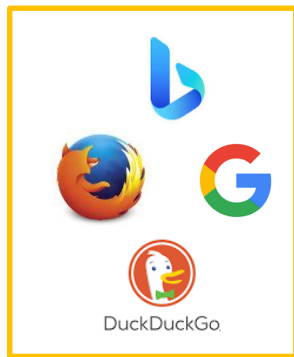
## Evolution of Consumer Large Language Models:

- LLMs have evolved from earlier **chatbots**, which have been around for decades.
- Essentially, they are computer algorithms that are **incredibly good at generating output** for given input. No magic, just a lot of data, math and matrices!
- Trained on **huge datasets**, they learn associations between words, and in doing so build a broad '**general knowledge**' about the world. They can be used to process **natural language**, understand context, and dynamically generate coherent responses from complex queries.
- Increasingly they have become more functional with **multimodal abilities**. They can even **run other programs** and **talk collaboratively to other LLMs**.

*Excellent overviews on Youtube:*

Andrej Karpathy: [Intro to Large Language Models.](#)

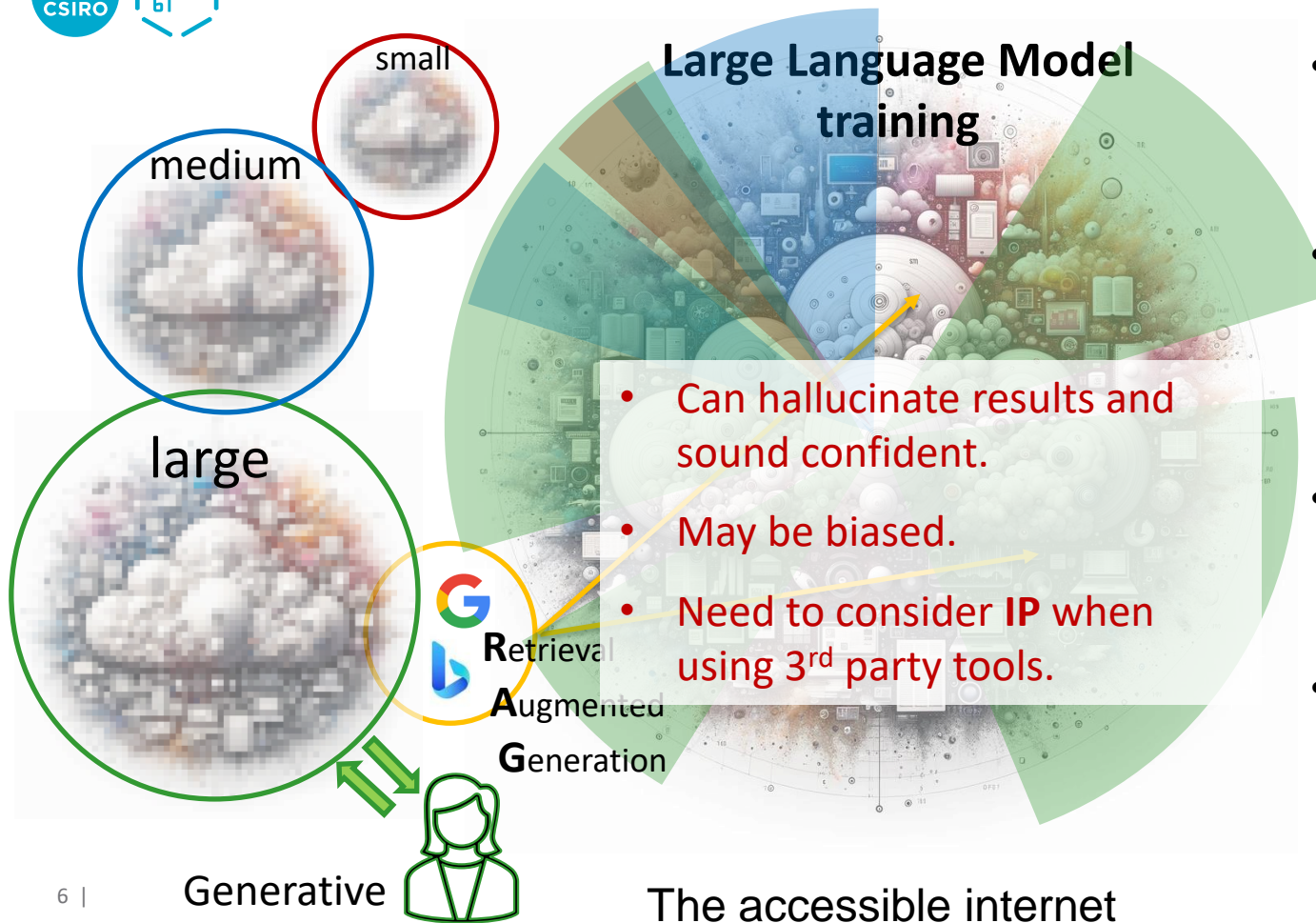
3Blue1Brown: [But what is a GPT?](#) and [Attention in transformers.](#)



## The problem with search:

- You have to know what you are looking for.
- You must interpret information from the provided webpage. (Also, ads & click bait!)
- The gatekeepers order search results based on algorithms/sponsorship. They watch you.
- Keyword and context ambiguity.

# Search vs Generative



## Generative AI:

- You can interact with LLMs using **natural language (NL)**.
- LLMs leverage **NL** to access interdisciplinary knowledge **across diverse domains**.
- They are multimodal and multilingual. Can be domain specific.
- Ever increasing capabilities: higher quality and **larger context windows**.



# Why use LLMs over Search Engines?

## Typical search engine query:

'Influenza reviews'

'How to code pairwise alignment of proteins'

'Antibiotics and drug resistance'

## Typical LLM interaction:

"What can you tell me about influenza? **Be detailed and summarize the main points.**"

"How would I code pairwise alignment of proteins? **Can you write an app in python and explain the steps of how it works?**"

"What is antibiotic resistance, - can you please give me a general overview? **Explain like I am 12.**"



# It is all in how you ask: The power of Chain of Thought prompting

If it takes **three hours to dry three towels** on a line, how long would it take to dry nine towels?

## ChatGPT:

If it takes three hours to dry three towels, then it takes  $3 \text{ hours} / 3 \text{ towels} = 1 \text{ hour/towel}$ .

To dry nine towels at the same rate:

Time = (number of towels)  $\times$  (time per towel)

Time = (number of towels)  $\times$  (time per towel)

It would **take 9 hours to dry nine towels** on the line, assuming the drying rate remains consistent.

If it takes three hours to dry three towels on a line, how long would it take to dry nine towels? **Think about this carefully before you answer and explain your reasoning.**

## ChatGPT:

Let's think about it step by step:

If it takes three hours to dry three towels, then it takes three hours for each towel to be fully dry. In other words, if you put three towels on a line, and come back in three hours, all three towels will be dry.

Now, if you add another three towels to the line, these new towels will also take three hours to dry. But since you're hanging them at the same time as the first three towels, all six towels will be dry in the same three hours.

Using the same reasoning, if you add yet another three towels (making it a total of nine towels), all nine towels will still take three hours to dry when hung up simultaneously.

So the answer is: it would still **take three hours to dry nine towels** when they're hung up at the same time on a long line.



# LLMs are bad at math and logic. Usually.

**nature**

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nature > articles > article

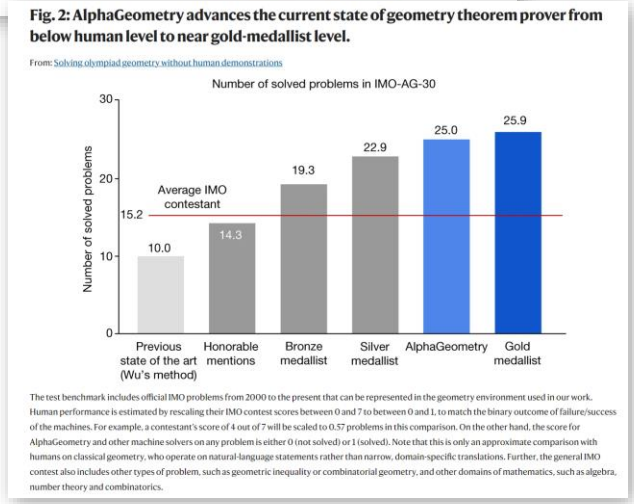
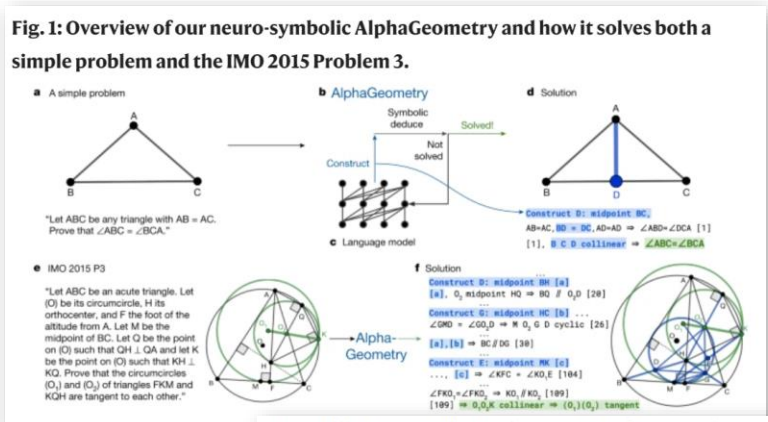
Article | [Open access](#) | Published: 17 January 2024

## Solving olympiad geometry without human demonstrations

[Trieu H. Trinh](#) [Yuhuai Wu](#), [Quoc V. Le](#), [He He](#) & [Thang Luong](#)

[Nature](#) **625**, 476–482 (2024) | [Cite this article](#)

149k Accesses | 900 Altmetric | [Metrics](#)



dolphin-2.7-mixtral-8x7b

MoE



Phi-3

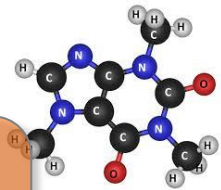
# Scientific LLMs, not just words:



```
..enha
incorp
adjacency knowledge,
ensuring that attention
calculations are
confined to neighboring
atoms only. Beyond
single-domain, MLM
extends to multi-domain
and multi-modal
approaches.
```

**Text based LLMs.**  
 BiomedGPT  
 Med-PaLM  
 Med-Gemini

**Molecular LLMs.**  
 DrugChat  
 ChemCrow



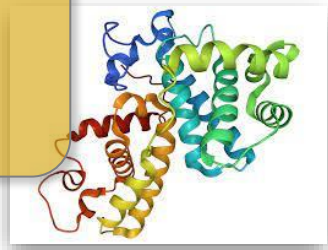
CN1C=NC2=C1C(=O)N(C(=O)N2)C



**Genomic LLMs.**  
 GenSLMs  
 Uni-RNA

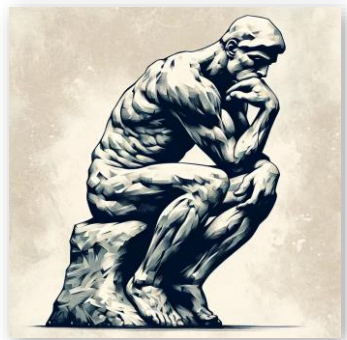
```
>ACTTGAATAGCCTAGCCGT
TAATCGCCTAGACGCTAAC
CGCAATGATTACA...
```

**Protein LLMs.**  
 ProGen2  
 ESM2, ProtNLM



```
MQIFVKTLTGKTITLEVEPSDTIENV
KAKIQDKEGIPPDQORLIFAGKQLED
GRTLSDYNIQRESTLHLVLRLLRGG
```

# Why do we need AI?



- 1) Managing Information Overload**
  - Analysing vast amounts of data and literature
- 2) Solving Complex, Interdisciplinary Problems**
  - Uncovering new connections; your personal ‘brainstorm buddy’
- 3) AI as a Personalized Tutor and Trainer**
  - Adapting to individual learning needs
- 4) Enhancing Cognitive Capabilities**
  - AI surpassing human performance



Garry Kasparov  
vs Deep Blue  
(1996)



Lee Sedol  
vs AlphaGo  
(2016)





## Capabilities of Gemini Models in Medicine

Khaled Saab<sup>o,†,1</sup>, Tao Tu<sup>o,†,1</sup>, Wei-Hung Weng<sup>o,†,1</sup>, Ryutarō Tanno<sup>o,2</sup>, David Stutz<sup>\*,2</sup>, Ellery Wulczyn<sup>\*,1</sup>, Fan Zhang<sup>\*,1</sup>, Tim Strother<sup>\*,1</sup>, Chunjong Park<sup>\*,1</sup>, Elahe Vedadi<sup>\*,1</sup>, Juanma Zambrano Chaves<sup>\*,1</sup>, Szu-Yeu Hu<sup>\*,1</sup>, Mike Schaekermann<sup>\*,1</sup>, Aishwarya Kamath<sup>\*,2</sup>, Yong Cheng<sup>\*,2</sup>, David G.T. Barrett<sup>\*,2</sup>, Cathy Cheung<sup>\*,1</sup>, Basil Mustafa<sup>\*,2</sup>, Anil Palepu<sup>\*,1</sup>, Daniel McDuff<sup>\*,1</sup>, Le Hou<sup>\*,2</sup>, Tomer Golany<sup>\*,4</sup>, Luyang Liu<sup>\*,1</sup>, Jean-baptiste Alayrac<sup>\*,2</sup>, Neil Houlsby<sup>\*,2</sup>, Nenad Tomasev<sup>\*,2</sup>, Jan Freyberg<sup>\*,1</sup>, Charles Lau<sup>1</sup>, Jonas Kemp<sup>1</sup>, Jeremy Lai<sup>1</sup>, Shekoofeh Azizi<sup>2</sup>, Kimberly Kanada<sup>1</sup>, SiWai Man<sup>1</sup>, Kavita Kulkarni<sup>1</sup>, Ruoxi Sun<sup>3</sup>, Siamak Shakeri<sup>2</sup>, Luheng He<sup>2</sup>, Ben Caine<sup>2</sup>, Albert Webson<sup>2</sup>, Natasha Latysheva<sup>2</sup>, Melvin Johnson<sup>2</sup>, Philip Mansfield<sup>1</sup>, Jian Lu<sup>1</sup>, Ehud Rivlin<sup>4</sup>, Jesper Anderson<sup>1</sup>, Bradley Green<sup>1</sup>, Renee Wong<sup>1</sup>, Jonathon Shlens<sup>2</sup>, Ewa Dominowska<sup>1</sup>, S. M. Ali Eslami<sup>2</sup>, Katherine Chou<sup>2</sup>, Claire Cui<sup>2</sup>, Oriol Vinyals<sup>2</sup>, Koray Kavukcuoglu<sup>2</sup>, James Manyika<sup>1</sup>, Jeff Dean<sup>1,2</sup>, Demis Hassabis<sup>2</sup>, Yossi Matias<sup>1</sup>, Dale Webster<sup>1</sup>, Joelle Barral<sup>2</sup>, Greg Corrado<sup>1</sup>, Christopher Semturs<sup>1</sup>, S. Sara Mahdavi<sup>\*,2</sup>, Juraj Gottweis<sup>\*,3</sup>, Alan Karthikesalingam<sup>\*,1</sup> and Vivek Natarajan<sup>†,1</sup>

<sup>o</sup>Co-first, <sup>\*</sup>Core, <sup>‡</sup>Technical Lead, <sup>†</sup>Senior Lead, <sup>1</sup>Google Research, <sup>2</sup>Google DeepMind, <sup>3</sup>Google Cloud, <sup>4</sup>Verily

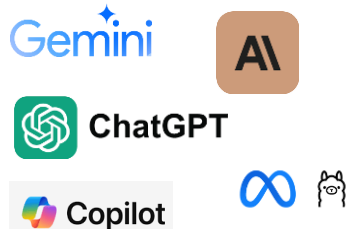
Excellence in a wide variety of medical applications poses considerable challenges for AI, requiring advanced reasoning, access to up-to-date medical knowledge and understanding of complex multimodal data. Gemini models, with their strong general capabilities in multimodal and long-context reasoning, offer exciting possibilities in medicine. Building on these core strengths of Gemini 1.0 and Gemini 1.5, we introduce *Med-Gemini*, a family of highly capable multimodal models that are specialized in medicine with the ability to seamlessly integrate the use of web search, and that can be efficiently tailored to novel modalities using custom encoders. We evaluate Med-Gemini on 14 medical benchmarks spanning text,

s.AI] 1 May 2024



# How: The AI toolbox. (as of early 2024\*)

## Generative AI.



## AI research assistants.



## AI coding assistants.



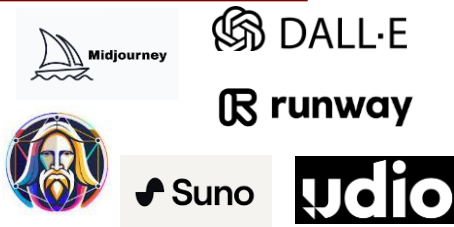
## AI structural biology.



## AI multi-agents.



## Image/video/music Generative AI.



## Custom GPTs Assistants.

- Mind Mentor**  
 A mentor bot encouraging critical thinking across various subjects.
- Scideator**  
 A formal, academic guide for scientific innovation.
- Text Razor**  
 I sharpen text for clarity and impact.
- MemChat**  
 A chatbot that creates downloadable 'memory' files from chat sessions for continuity.



# **How:** Demo of ChatGPT / Gemini / Claude 3 - or, “What could go wrong?”

# How: Demo of GPTs assistants



**Aldeator:** A tool for understanding and strengthening ideas with insightful dialogue.

<https://chat.openai.com/g/g-4UrZNpH50-aideator>



**Paper Mache:** Reviews uploaded Scientific Papers and provides a summary and critique.

<https://chat.openai.com/g/g-uJvQlkk0d-paper-mache>



**Meeting Scribe:** I create meeting summaries and action items from transcripts.

<https://chat.openai.com/g/g-0aWDdYa28-meeting-scribe>

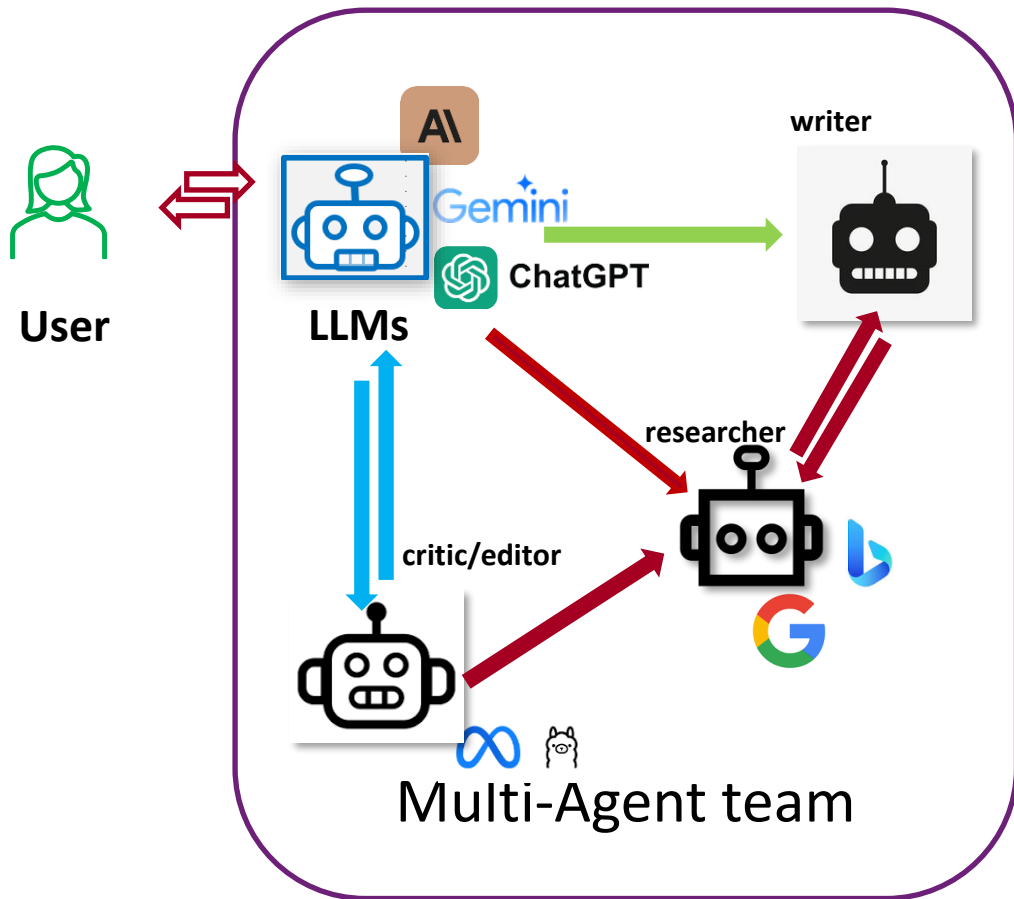


**Text Razor:** I sharpen text for clarity and impact.

<https://chat.openai.com/g/g-FExztI0NU-text-razor>



# LLMs as Agents.



## Multi-Agent Frameworks:





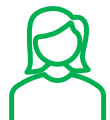


# LLMs as Agents.

```
researcher = Agent(  
    role='Senior Researcher',  
    goal='Perform comprehensive scientific research on the given topic: {topic}. Use reliable sources  
and critically evaluate the information found.',  
    verbose=True,  
    memory=True,  
    backstory="""As a highly skilled researcher, you provide in-depth and comprehensive reports.  
Your research begins with finding relevant articles for the subject matter and reading their  
content. Provide at least TEN references which MUST be cited at the end of the report using  
proper citation format.  
The report should be structured with an introduction, background, main findings, discussion,  
conclusion, and references sections. You will provide your report to the reviewer who will provide  
constructive feedback, and you will use this feedback to improve your article."""  
    tools=[search2, website_rag],  
    llm=gpt4,  
    allow_delegation=True
```



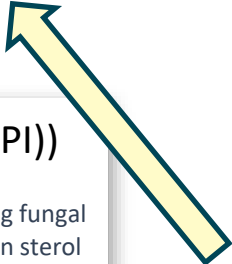
# Custom AI agent research teams.



Find new protein antibiotic targets for:  
*Candida albicans*



Project Manager



Researcher Agent



Research\_task  
gpt-4



Reports/research\_report.md



Reviewer Agent

Review\_task  
gpt-4

Reports/peer\_review.md



Researcher Agent

Rewrite\_task  
gpt-4

Reports/revised\_research\_report.md



Writer Agent



Strategy Agent

Reports/scientific article.md

Reports/research\_strategy\_proposal.md

Reports: (approx. 3-4 minutes, ~ \$1 (using OpenAI API))

- Ergosterol Biosynthesis Pathway:** This pathway is essential for maintaining fungal membrane integrity. While ERG11 is already targeted by azoles, ERG6, involved in sterol biosynthesis, shows promise based on preliminary studies (Watanabe et al., 2012).
- Cell Wall Integrity Pathway:** Proteins such as glucan synthases, crucial for cell wall synthesis and remodeling, are potential targets. Their disruption can lead to increased susceptibility to osmotic stress and antifungal agents.
- Biofilm Formation:** Proteins like Biofilm-associated protein (Bap) and adhesins such as Als3 are vital for biofilm formation and maintenance, contributing significantly to antifungal resistance

\* References legit and relevant. Pop science article and strategy report high level.



# The AI tool chain:



Report:

1. Ergosterol Biosynthesis Pathway:
2. Cell Wall Integrity Pathway:
3. Biofilm Formation:

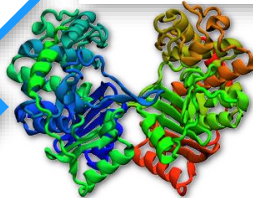


Bioinformatics

Gemini Med-Gemini

Galaxy

Alphafold



Protein binder

RF diffusion

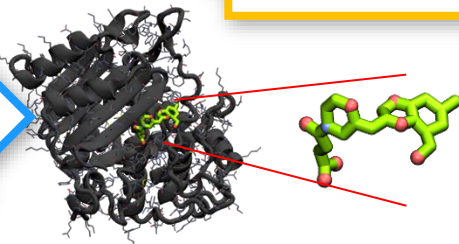
Protein MPNN

Experimental validation



RosettaFold AA

Pocket2Mol



Small molecule inhibitor



# The AI tool chain:

## nature

Article | [Open access](#) | [Published: 20 December 2023](#)

### Autonomous chemical research with large language models

[Daniil A. Boiko](#), [Robert MacKnight](#), [Ben Kline](#) & [Gabe Gomes](#)

[Nature](#) **624**, 570–578 (2023) | [Cite this article](#)

## nature chemical engineering

Article | [Open access](#) | [Published: 11 January 2024](#)

### Self-driving laboratories to autonomously navigate the protein fitness landscape

[Jacob T. Rapp](#), [Bennett J. Bremer](#) & [Philip A. Romero](#)

[Nature Chemical Engineering](#) **1**, 97–107 (2024) | [Cite this article](#)



Robotlabs?

Autonomous research?

Google RT-2 ?





# What possibly could go wrong?



Contents lists available at [ScienceDirect](https://www.sciencedirect.com)

## Surfaces and Interfaces

journal homepage: [www.sciencedirect.com/journal/surfaces-and-interfaces](https://www.sciencedirect.com/journal/surfaces-and-interfaces)



The three-dimensional porous mesh structure of Cu-based metal-organic-framework - aramid cellulose separator enhances the electrochemical performance of lithium metal anode batteries

Manshu Zhang<sup>a,1</sup>, Liming Wu<sup>a,1</sup>, Tao Yang<sup>b</sup>, Bing Zhu<sup>a</sup>, Yangai Liu<sup>a,\*</sup>

<sup>a</sup> Beijing Key Laboratory of Materials Utilization of Nonmetallic Minerals and Solid Wastes, National Laboratory of Mineral Materials, School of Materials Science and Technology, China University of Geosciences, Beijing100083, China

<sup>b</sup> College of Materials & Environmental Engineering, Hangzhou Dianzi University, Hangzhou 310036, China



## Constant vigilance.

## 1. Introduction

Certainly, here is a possible introduction for your topic: Lithium-metal batteries are promising candidates for high-energy-density rechargeable batteries due to their low electrode potentials and high theoretical capacities [1,2]. However, during the cycle, metal batteries are promising candidates for high-energy-density rechargeable batteries due to their low electrode potentials and high theoretical capacities [1,2]. However, during the cycle, dendrites forming on the lithium metal anode can cause a short circuit, which can separator helps to prevent the formation of reactive species that can further promote dendrite growth. Researchers are actively exploring different materials and designs for separators to enhance their mechanical strength and chemical stability. These efforts aim to create

metal batteries are promising candidates for high-energy-density rechargeable batteries due to their low electrode potentials and high theoretical capacities [1,2]. However, during the cycle, dendrites forming on the lithium metal anode can cause a short circuit, which can

separator helps to prevent the formation of reactive species that can further promote dendrite growth. Researchers are actively exploring different materials and designs for separators to enhance their mechanical strength and chemical stability. These efforts aim to create

# Recap: How to get more from your ‘cognitive co-pilots’.

- Take time to set the context of your questions:  
**Be conversational.** Use **chain of thought** prompting.
- If something is not clear, ask for clarification. Fill your gaps of knowledge.  
**Ask to test your understanding.** Don't be lazy.
- **Check everything.** Ask for sources.
- When brainstorming, remember to **ask for additional ideas** and **critique of your own.**
- Be **mindful of IP and privacy** when using tools.



nature

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[nature](#) > [perspectives](#) > article

Perspective | [Published: 06 March 2024](#)

## Artificial intelligence and illusions of understanding in scientific research

[Lisa Messeri](#)  & [M. J. Crockett](#) 

[Nature](#) **627**, 49–58 (2024) | [Cite this article](#)

**18k** Accesses | **3** Citations | **697** Altmetric | [Metrics](#)



# The Future of AI in Science.

- **Large commercial investments and rapid developments:**
  - Hard to predict what new capabilities will exist next week:  
Be **agile**. **Don't** believe all the **hype**.
- **Transformative potential:**
  - New capabilities will radically alter how we process and interpret data.  
ie) multimodal and data analytics in OpenAI and Gemini models
  - Can we use AI to drive autonomous research (via agents/robotics) and software development?
- **Big questions remain on long term consequences of using AI tools:**
  - Do we **lose cognitive and critical** thinking skills?
  - Do we still need to be domain experts?
  - How much do we trust the output?



Thank You

## Where to next?

### Resources:



National  
Artificial  
Intelligence  
Centre

- AI training
- Responsible AI
- Industry networking



- Matt Wolfe
- Matthew Berman
- AI explained

**ANTHROPIC**

Prompt library:

<https://docs.anthropic.com/claude/prompt-library>



[michael.kuiper@csiro.au](mailto:michael.kuiper@csiro.au)