





Artificial intelligence and the future of science





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UNESCO Chair on the Ethical Governance of Artificial Intelligence, IPPT PAN, Warsaw 15.12.2025

Towards autonomous ethical AI agents

- 1. Few thoughts on AI: computing, intelligence, cognition.
- 2. Superintelligence and exponential growth.
- 3. Al4Science autonomous agentic Al science factories.
- 4. Ethical side: Al too human?



should we be more afraid that AI will turn against us, or that we turn against AI and others will enslave us?

ChatGPT << AI, 150-300 papers in the <u>arxiv.cs.ai</u> each day! NeurNIPS 2025, 15 000 papers, 5 290 accepted.





Duch W, Diercksen GHF (1994) <u>Neural networks as tools to solve problems in physics and chemistry</u>. Computer Physics Communication **82**: 91-103

MAGAZINES























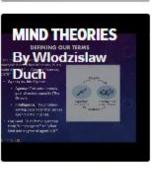




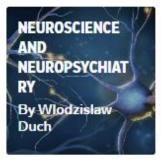




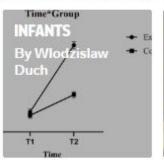
























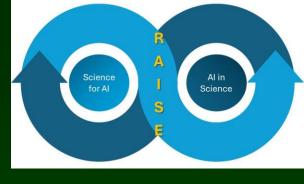




My Flipboards

EU RAISE Projects

A European Strategy for Artificial Intelligence in Science. Paving the way for the Resource for AI Science in Europe (RAISE).



Announced at AI in Science Summit in Copenhagen on 3-4.11.2025 with pilot funding 108 M EUR. In 2018 communication from the EU Commissison promised 20 B EUR/year -;)

RAISE is launched as a virtual European institute that pools, aligns and coordinates essential AI resources, including computational power, data, excellence and talent, and research funding, across the EU, Member States and private sector. It will support the development of AI systems beyond the current state of the art, that are ethical, explainable, transparent, accountable, reliable, safe, human-centric and aligned with human rights and societal values.

81% of researchers have concerns relating to AI models (ethics, accuracy, security/privacy, and/or lack of transparency) and 63% to the lack of guidelines, hindering the adoption of AI (survey . The Commission will continue to promote the "ethics by design" approach and develop different resources with the scientific community (training, tools, etc.).

The <u>European Group on Ethics in Science and New Technologies</u> (EGE) will evaluate this program. <u>Nauka o Al, Al dla nauki</u>.

Defining intelligence

What is really important: not how we call it but what it can do!

If we have **effective** algorithms we can write programs, no need for Al.

No effective algorithms? Intelligence is needed.

Intelligence: ability to solve problems where no effective algorithms are known. Al does it using some hardware, humans use wetware.

What cannot be successfully programmed but can be learned from experience may be replicated in a supervised way, discover in unsupervised way, or strategies may be developed using reinforcement learning.

Humans are megalomaniacs and believe in magic in their wetware, but understanding == compression of complexity into coherent patterns.

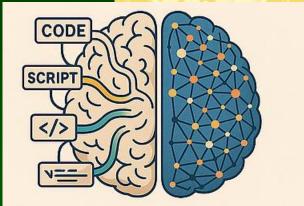
Transferring disorganized data => structure.

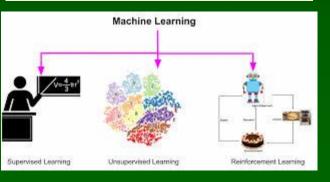
Al cannot always be perfect, but it can be better than humans.

Hardware could be biological, electronic, photonic, spintronic, atomic ...









More substrates for thinking

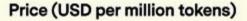


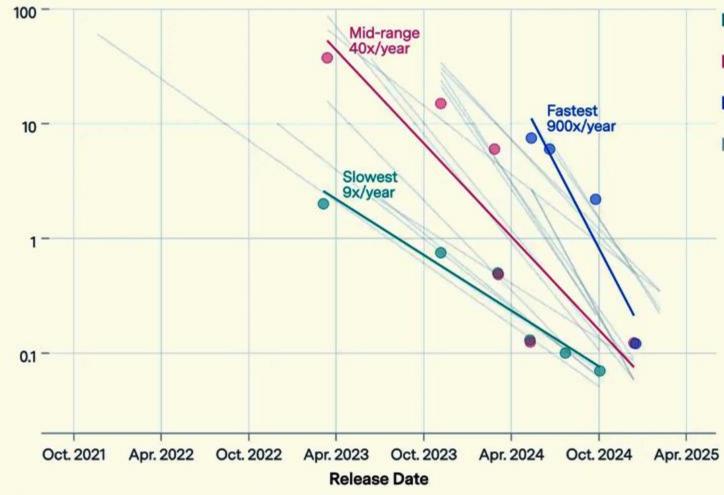


New hardware has no constraints of wetware. Photonics: <u>Taichi chiplet</u> 160 TOPS/W, <u>Q.ant</u> photonic chip, <u>Lightmatter 3D Photonic</u> 500-1000 TOPS/W. <u>Groq Linear Processing Unit</u> LPU, 400 TOPS/W. Cerebras, CIMs, spintronics, neuromorphic computing, Cortical Labs organoids CL1 <u>800k cells chip</u>. LLM inference <u>cost fall between 9-900x/year</u>, depending on the task (<u>Epoch.ai</u>). Energy may soon not be a problem. Should our AI factories use classical hardware?

LLM inference prices have fallen 9x to 900x/year, depending on the task







Data source: Epoch Al, Artificial Analysis

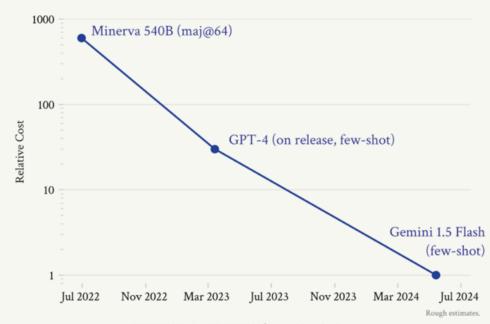
CC-BY

 GPT-3.5 Turbo level or better on general knowledge (MMLU)

- GPT-4 level or better on Ph.D. level science questions (GPQA)
- GPT-40 level or better on Ph.D. level science questions (GPQA)
- Other benchmarks and performance levels

Who needs GWs?

Relative (inference) cost of ~50% performance on the MATH benchmark



SITUATIONAL AWARENESS | Leopold Aschenbrenner

Embedding + attention = transformers

Word2Vec, Glove, FastText: embedding of words as vectors in the parameter space, preserving similarity.

Each word is encoded in a large number of contexts.

Transformer model <u>published</u> by <u>Google in June 2017</u>: Attention is all you need, started the generative AI era.

A key concept of GPT is self-attention to relationships between tokens, linking each token to other tokens.

Vectors of concepts that are semantically related become similar to each other

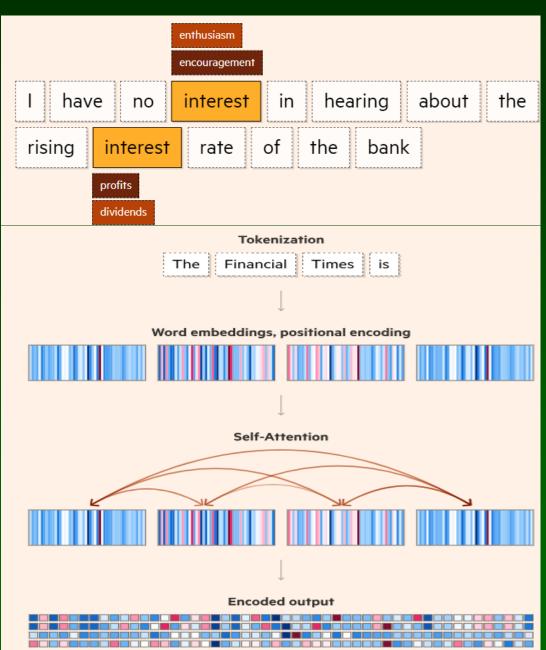
=> GPT interprets inputs using meaningful associations.

Associative thinking: creative, heuristics for reasoning.

Matykiewicz P, Pestian J, Duch W, and Johnson N. (2006)

<u>Unambiguous Concept Mapping in Radiology Reports:</u>

<u>Graphs of Consistent Concepts</u>, AMIA Ann. Symp Proc. 1024.



Transformers and spreading activation

Predictive AI: search + heuristics, supercalculator.

Generative AI: spreading activation networks, binding relevant information.

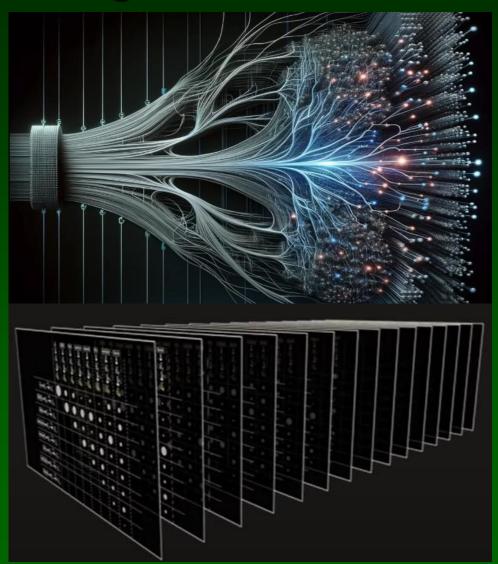
GPT = Generative Pre-trained Transformer

Input data ⇒ tokens ⇒ embed in vector space, preserve similarity of meaning (semantics) in different contexts.

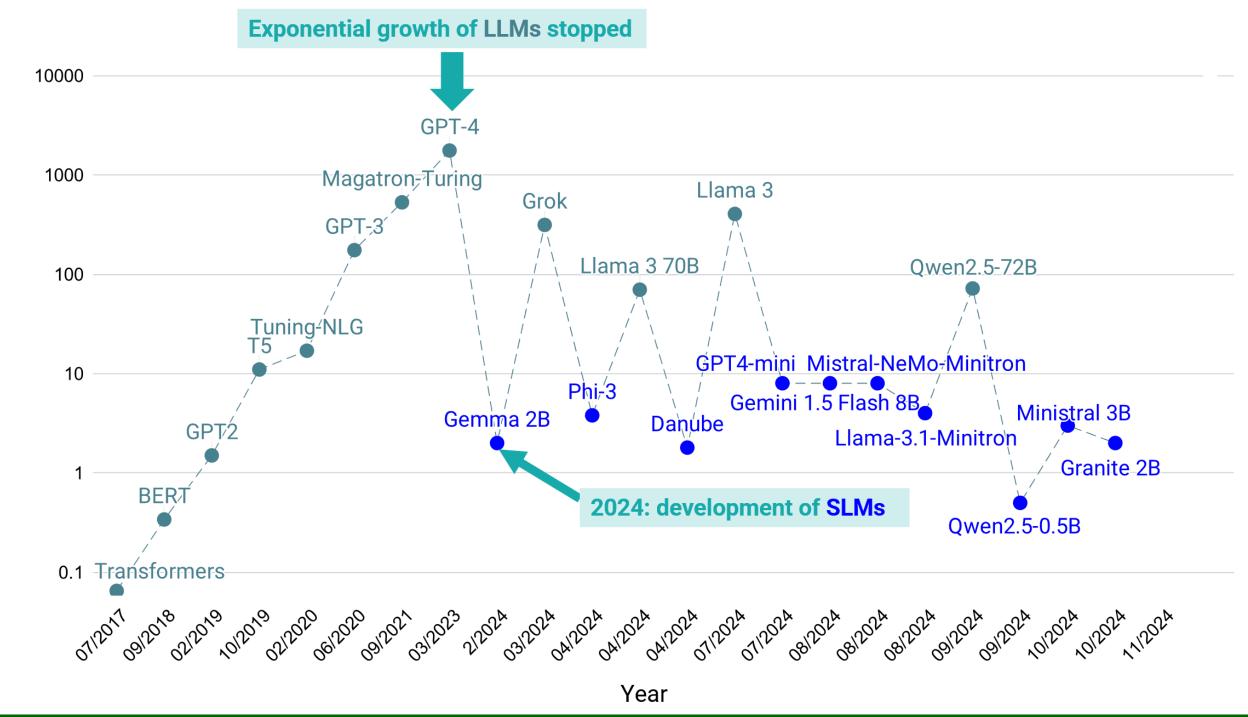
Analyze relations between tokens, create structured knowledge graphs.

LLM visualization https://bbycroft.net/llm

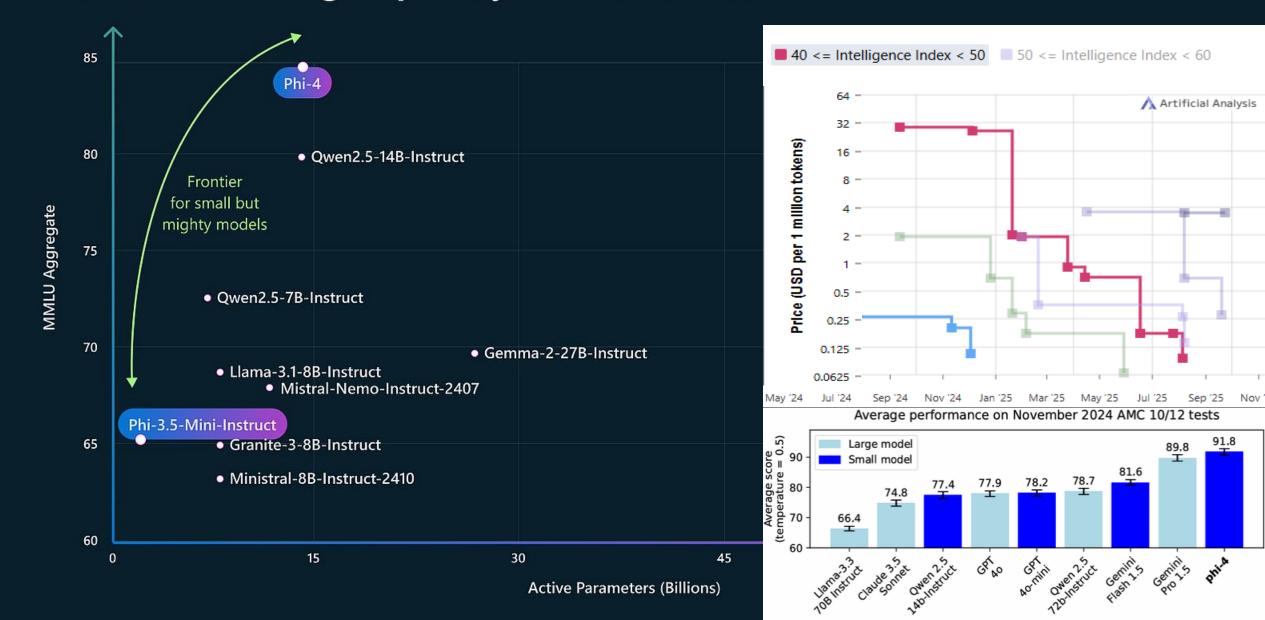
Over 51 565 variants of open-source LLMs, over 3000 for fine-tuning (<u>LLM Explorer</u>, 14/12/25).



Processing clinical text with domain-specific spreading activation methods. US Patent US8930178B2 (1/2015) Duch W, Matykiewicz P, Pestian J, Towards Understanding of Natural Language: Neurocognitive Inspirations. 2007



Phi-4 offers high quality results at a small size



Prompt optimization

GPTs/LLMs need Medprompt to achieve SOTA performance on a wide range of medical problems. Microsoft Research tools for thought, promptions. Best prompt libraries.

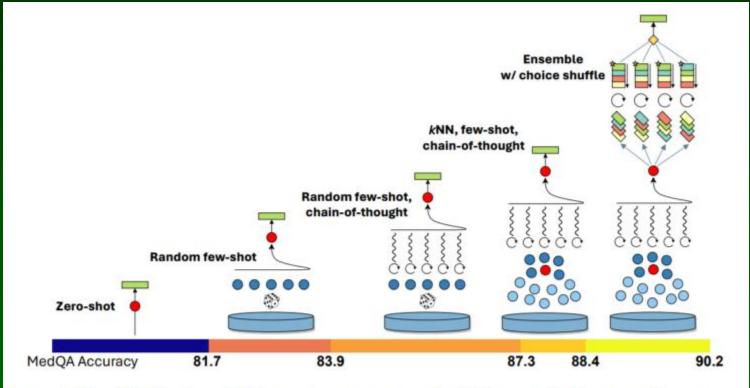
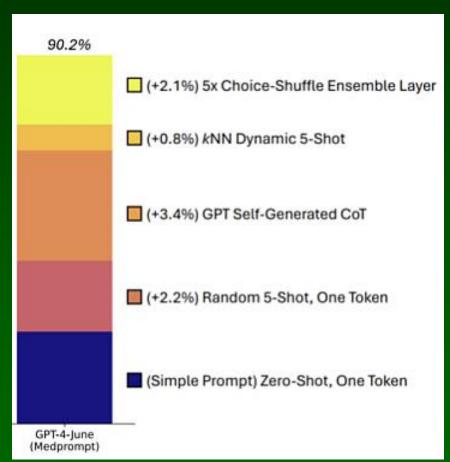


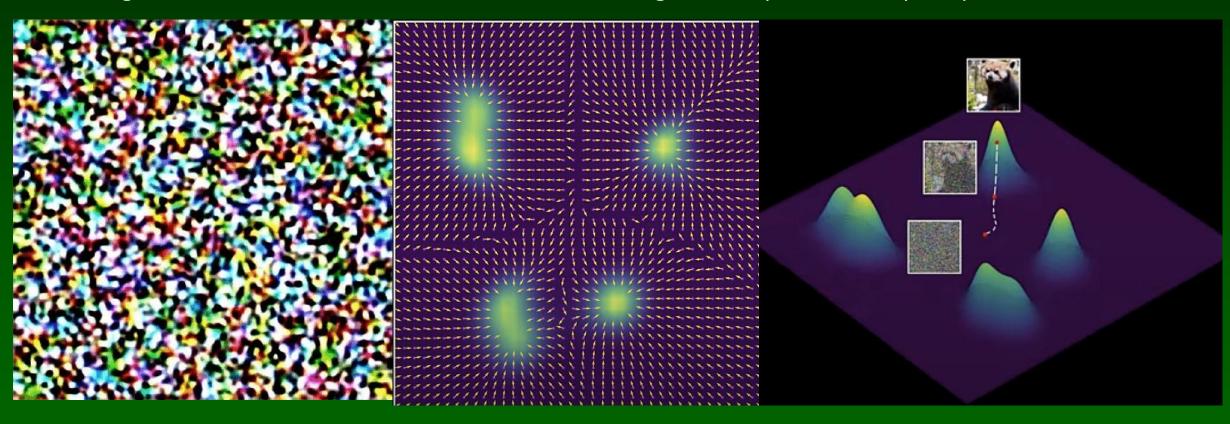
Figure 4: Visual illustration of Medprompt components and additive contributions to performance on the MedQA benchmark. The prompting strategy combines kNN-based few-shot example selection, GPT-4–generated chain-of-thought prompting, and answer-choice shuffled ensembling (see details in



GPT finds associations: first thing that comes to mind/network. Needs verification, reasoning.

Diffusion models

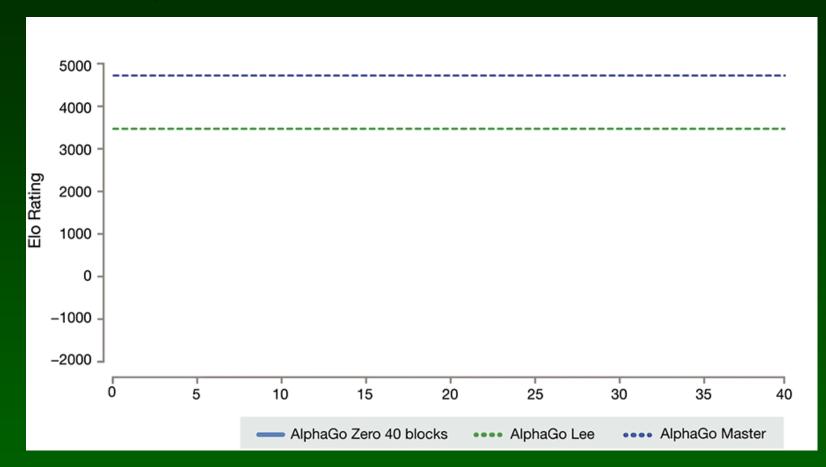
Almost all image/audio/video systems are based on diffusion. A few sentence generation are based on continuous diffusion. Sometimes we try to complete a sentence, but sometimes it comes all at once. Create gradient field towards attractor basins where images/concepts linked to prompts are stored.



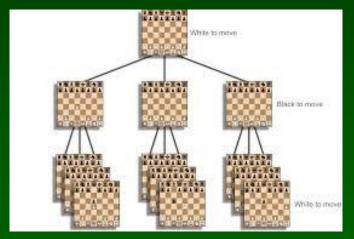
See videos at the ode-pth-first YT channel. Diffusion has deep roots in statistical physics.

Nobelization of Neural Networks: Deep Roots and Insane Future of Neural Networks (INNS 12/2024).

AlphaGo Zero and verifiable rewards (RLVR)



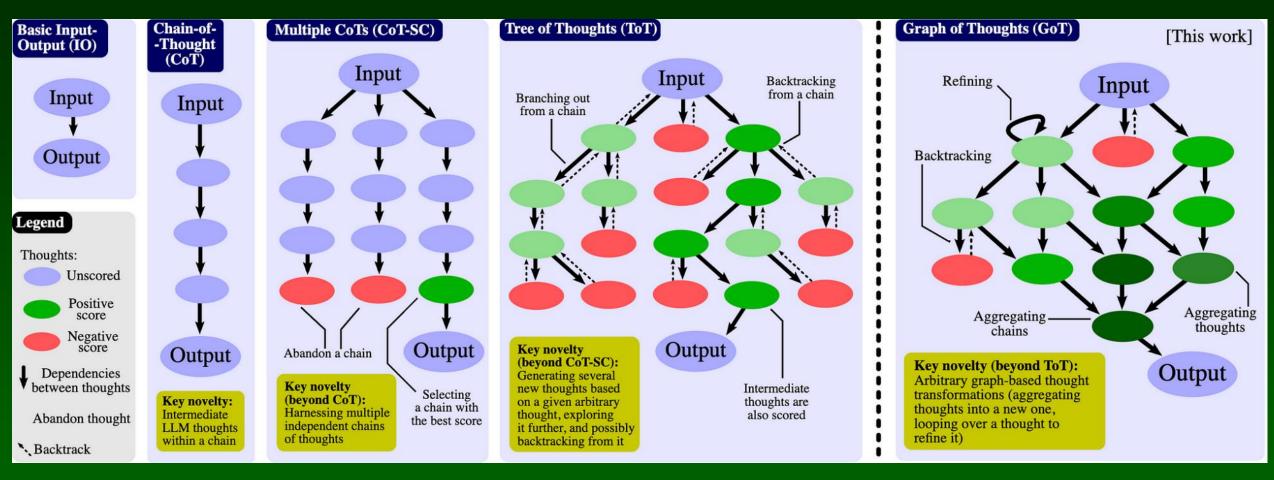
1997, Deep Blue-Kasparov. 2016, AlphaGo-Lee Sedol 2017, Alpha GoZero 2017, Poker, Dota 2; 2019, Starcraft II, 2022 Stratego, Diplomacy



Superhuman level in Go. Best humans 3,600–3,860 ELO, KataGO over 6000 ELO, playing against itself! Human knowledge becomes irrelevant, decreasing Al competence! Can we do it in other domains? Reinforcement learning with Verifiable Rewards, RLVR continuous self-improvement. **Shocking news:** Ruoss ... & Genewein, T. (2/2024). *Grandmaster-Level Chess Without Search*.

270M parameter transformer model, 1-step intuitive decisions! Like in Blitz Chess.

Reasoning – cognitive inspirations



Associations: input => output.

Chain of thought (CoT): step by step.

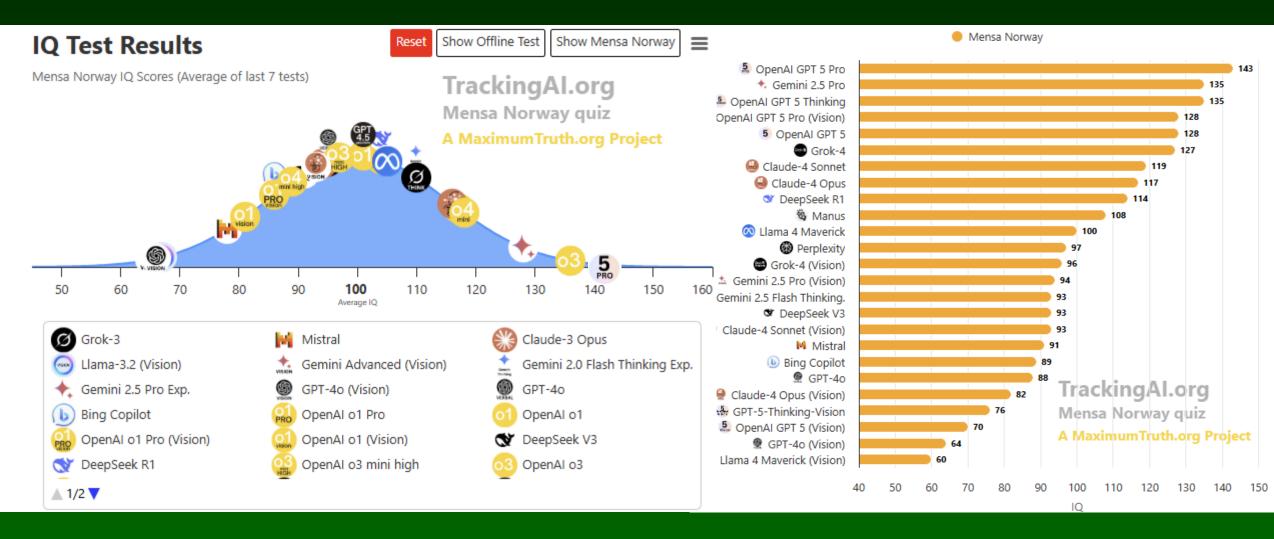
This is GOFAI! LLM associations in heuristic search.

<u>Tree of Thoughts</u> (ToT): <u>parallel thinking</u> via RL.

Graph of Thoughts (GoT): like human reasoning.

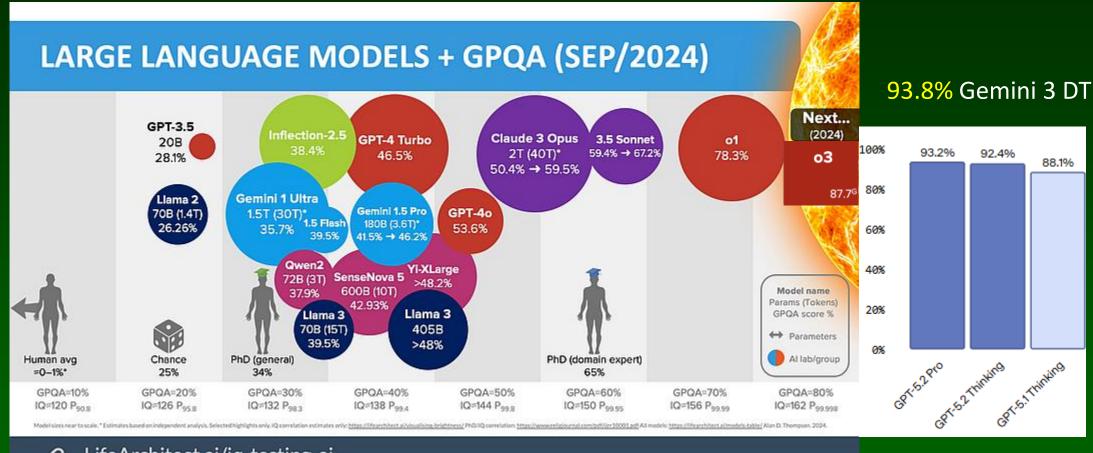
Sketch-of-Thought: adaptive cognitive-Inspired sketching

MIQ of AI



At the beginning of the 2024 highest results were < 100 points. Gemini 3 Pro, GPT 5.1 Pro > 140. 29.09.2025: Claude Sonnet 4.5 shows 30+ hours of autonomous coding.

GPQA benchmark



LifeArchitect.ai/iq-testing-ai

Rein, D et al. (2023). *GPQA: A Graduate-Level Google-Proof Q&A Benchmark*. arXiv:2311.122 448 extremely difficult questions: highly skilled non-expert validators reach 34% accuracy with >30 minutes of web access, experts pursuing PhDs in the corresponding domains reach 65%-74%.

International Collegiate Programming Contest (ICPC)

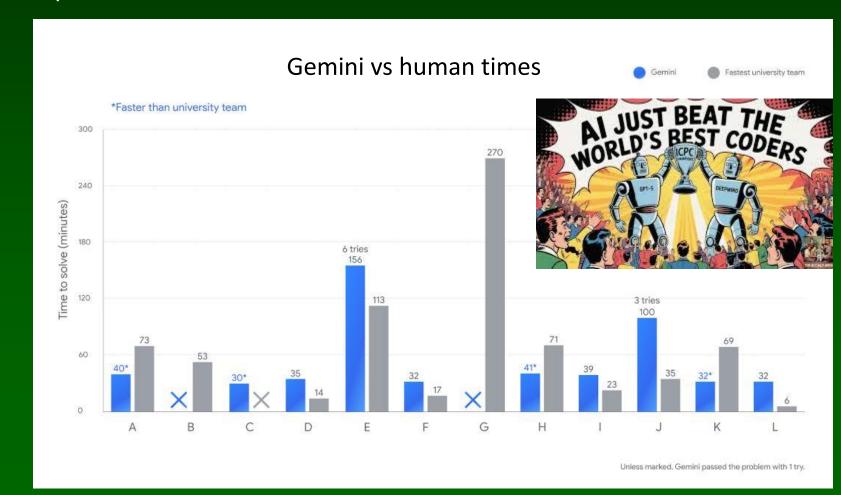
9/2025: teams from 139 universities in 103 countries participated in the ICPC finals.

Team: 3 students. Task: solve 12 algorithmic problems within 5 hours. Cutting-edge algorithms: graph theory, number theory, dynamic programming, combinatorial optimization, network flow ... Ranking depends on the number of problems solved and the time taken.

3 human teams, from Saint Petersburg State University, the University of Tokyo, Beijing Jiaotong, solved 11 problems.

GPT-5 solved all 12 problems, 11 on the first try, last on 9th submission, 12/12.

Gemini 2.5 Deep Think solved 10/12, including problem that no human team could solve.



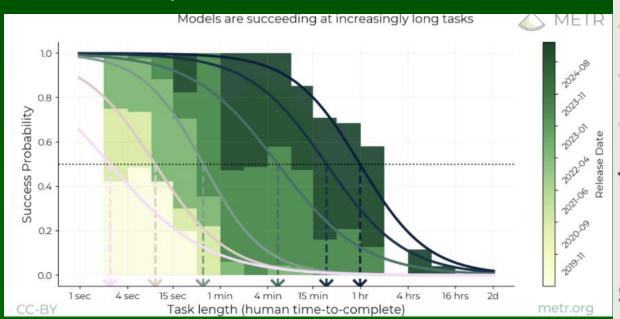
Long tasks

Measuring Al Ability to Complete Long Tasks.

Al performance in terms of the length of tasks Al agents can complete. GPT5: 2h15m-4.5h.

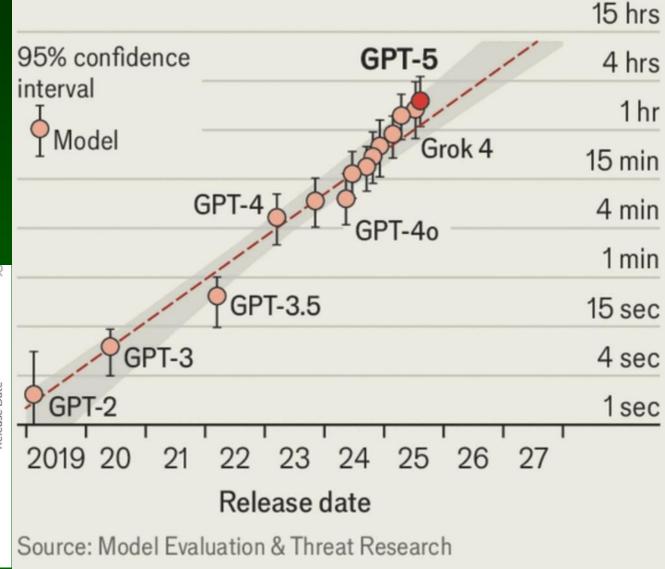
This metric has been consistently exponentially increasing over the past 6 years, with a doubling time of less than 7 months.

In less than a decade AI agents should complete independently a large fraction of tasks that take humans days or weeks.



Software-engineering tasks where selected LLM achieves a 50% success rate

Average task duration for humans, log scale



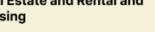
GDPval real work test

Most benchmarks do not show real value of AI models.

GDPval is based on real-world work from 44 occupations.

In pairwise comparisons some AI models approach parity with industry experts (av. 14 years experience) on the GDPval gold subset (220 tasks). Win rate of GPT 5.2 is 60%, with ties 74%.

Real Estate and Rental and Leasing



- Concierges
- · Real Estate Sales Agents
- · Real Estate Brokers
- · Counter and Rental Clerks
- · Property, Real Estate, & Community Association Managers

Professional, Scientific, and Technical Services

- Software Developers
- Lawyers
- Accountants & Auditors
- Computer & Information Systems Managers
- Project Management Specialists

Government



- · Recreation Workers
- Compliance Officers

Assistance

Registered Nurses

· Nurse Practitioners

Support Workers

- · First-Line Supervisors of Police and Detectives
- · Administrative Services Managers

Health Care and Social

· Medical & Health Services Managers

· Child, Family, and School Social Workers

Manufacturing



- · Mechanical Engineers
- Industrial Engineers
- · Buyers & Purchasing Agents
- · Shipping, Receiving, & Inventory Clerks
- · First-Line Supervisors of Production and Operating





- · Customer Service Representatives
- Financial Managers
- Personal Financial Advisors
- Securities. Commodities & Financial Services



- Retail Trade Pharmacists
- · General and Operations Managers
- · Private Detectives & Investigators
- · First-Line Supervisors of Retail Sales Workers

Wholesale Trade



- Sales Managers
- · Order Clerks
- Sales Representatives, Wholesale & Manufacturing. Technical & Scientific Products

First-Line Supervisors of Office & Administrative

· Medical Secretaries & Administrative Assistants

- Sales Representatives, Wholesale & Manufacturing. Except Technical & Scientific Products
- First-Line Supervisors of Non-Retail Sales Workers

Finance and Insurance

- · Financial & Investment Analysts

- Sales Agents

Information



- · Producers & Directors
- · Film & Video Editors
- Editors
- · News Analysts, Reporters, & Journalists
- · Audio and Video Technicians



Ekspe



Artificial Intelligence-Enabled Medical Devices

11/2025: AI/ML-Enabled FDA approved 1247 Medical Device List.

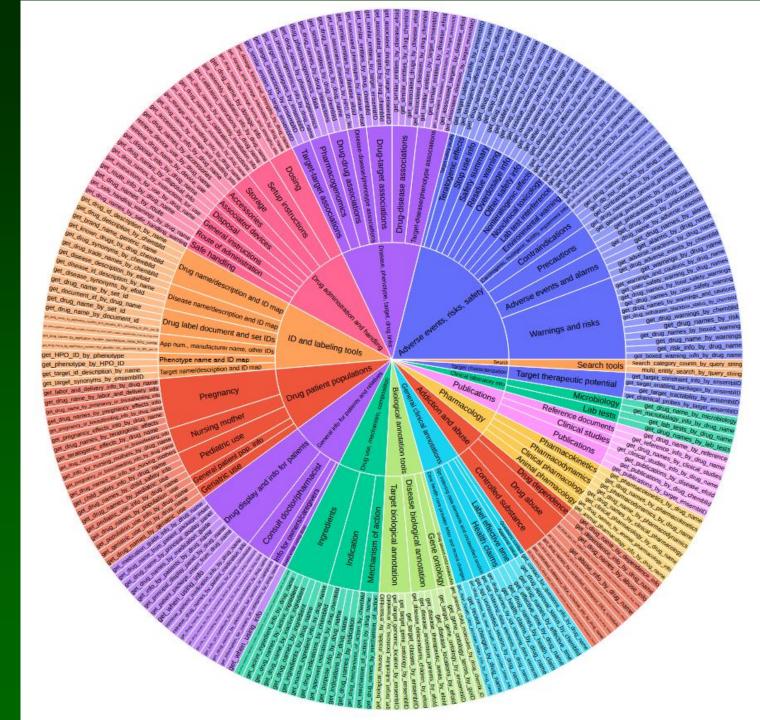
- 956 Radiology
- 125 Cardiovascular
- 56 Neurology
- 22 Anesthesiology
- 19 Hematology
- 17 Gastroenterology-Urology
- 10 Ophthalmic
- 43 Remaining



TOOLUNIVERSE: 211 biomedical tools

Gao, S. ... & Zitnik, M. (3/2025). <u>TxAgent</u>: An Al Agent for Therapeutic Reasoning Across a Universe of Tools.

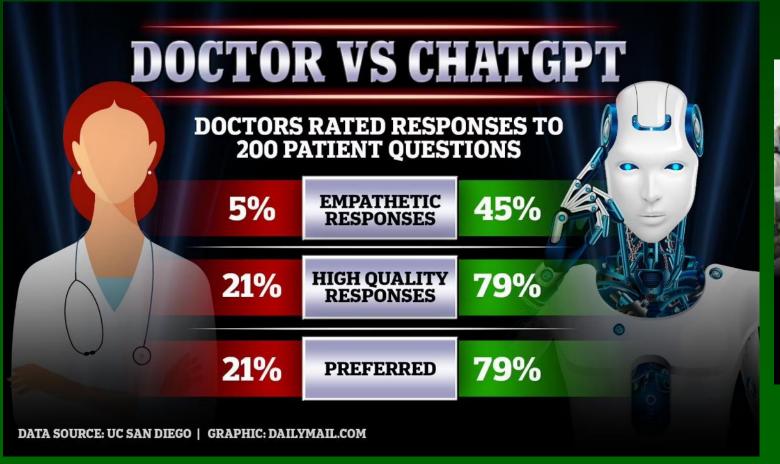




Do you really want a human doctor?

• Goh, E. +15 coauthors (10/2024). Large Language Model <u>Influence on Diagnostic Reasoning</u>: A Randomized Clinical Trial. *JAMA Network Open*, 7(10), e2440969–e2440969.

50 physicians, median diagnostic reasoning score was 74% (IQR, 63%-84%), with the help of GPT4 76% (IQR, 66%-87%) and LLM alone 92% (IQR, 82%-97%).





Tsinghua Hospital Simulacrum

Simulacrum-based Evolutionary Agent Learning (SEAL).

Hospital with 25 GPT-3.5 agents, 16 functional areas, 21 clinical departments, covering 339 diseases, simulates the entire process of treating disease.

Autonomous agents as patients, nurses and doctors. Agent doctors learn accumulating experience.

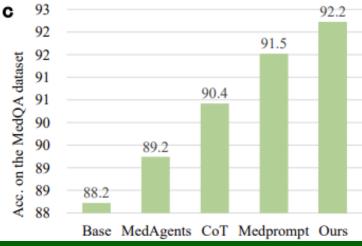
Evaluation: correct medical examination, diagnosis, and treatment plan recommendation.

After thousands of patients, Agent-Doctor reaches high competence without any manually labeled training data.

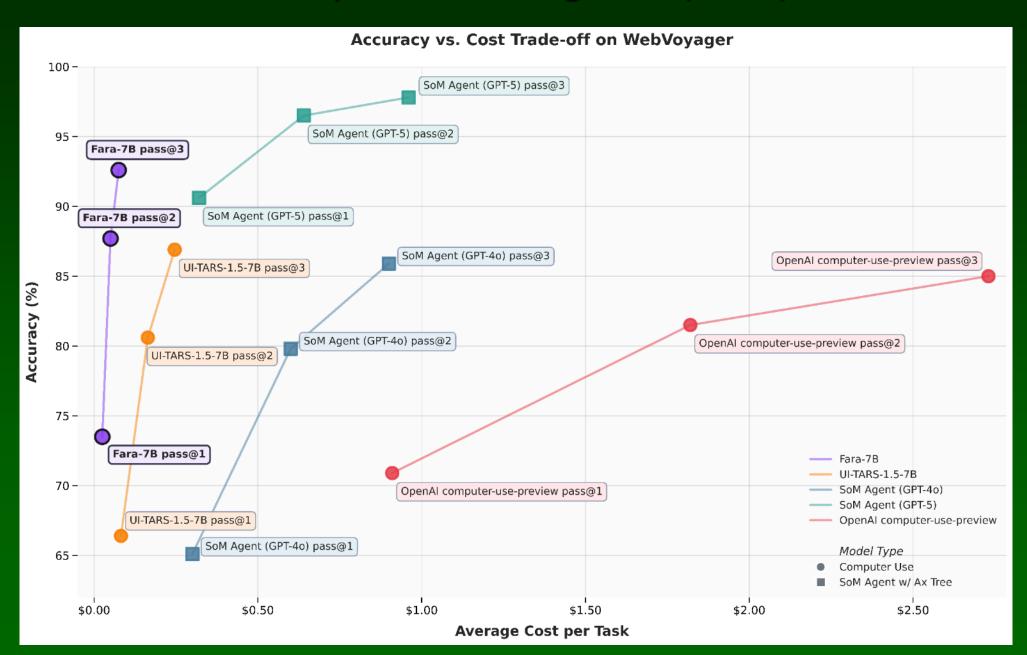
Li J. et al. (5/2024). <u>Agent Hospital</u>: A Simulacrum of Hospital with Evolvable Medical Agents.

5/2025: <u>Tsinghua Al Agent Hospital</u> was opened, strategic initiative transforming healthcare delivery, clinical education, and medical research through deeply integrated Al systems with agents trained in >20 specialties. Goal: training a new generation of "Al-collaborative physicians".



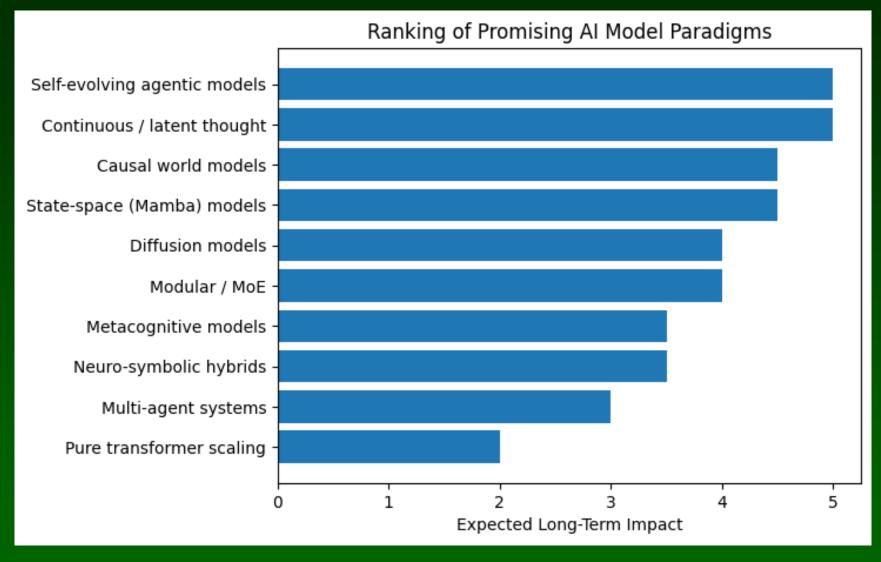


Computer Use Agents (CUA)



State-of-the-Art

Ranking of new Al models



Combination: State-space dynamics + latent reasoning + causal models + self-evolving agents.

Efficient/latent reasoning

Al Just Hit a Wall.
This Model Smashed
Right Through It

Explicit CoT to Implicit CoT

Latent Reasoning (§3.1.4)

Latent Space Representations Implicit-KD (Deng et al., 2023), Distill2-to-1 (Yu et al., 2024), CODI (Shen et al., 2025c), LightThinker (Zhang et al., 2025a), CCoT (Cheng & Van Durme, 2024), HCoT (Liu et al., 2024c), SoftCoT (Xu et al., 2025c), SI (Deng et al., 2024), RELAY (Yu et al., 2025a), Reasoning with Latent Thoughts (Saunshi et al., 2025)

Implicit-KD (Deng et al., 2023), Distill2-to-1 (Yu et al., 2024), CODI (Shen et al., 2025c), LightThinker (Zhang et al., 2025a), CCoT (Cheng & Van Durme, 2024), HCoT (Liu et al., 2024c), SoftCoT (Xu et al., 2025c), SI (Deng et al., 2024), RELAY (Yu et al., 2025a), Reasoning with Latent Thoughts (Saunshi et al., 2025), Planning-Token (Wang et al., 2024c), Filler-Token (Pfau et al., 2024), Coconut (Hao et al., 2024), Heima (Shen et al., 2025a), Token Assorted (Su et al., 2025), Disentangling-Memory-and-Reasoning (Jin et al., 2024a)

Hao S et al. Training Large Language Models to Reason in a Continuous Latent Space. Chain of Continuous Thought model (Coconut), emergence of advanced reasoning patterns.

Feng S, Fang G, Ma X, Wang X. 2025

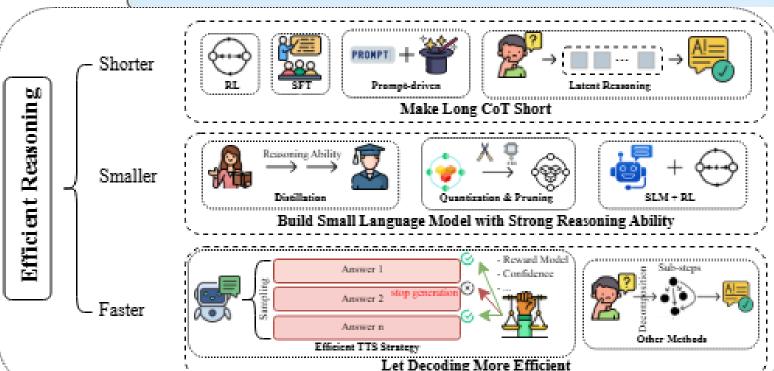
<u>Efficient Reasoning Models</u>: A Survey.

Github papers on efficient reasoning.

Github LatentCoT-Horizon

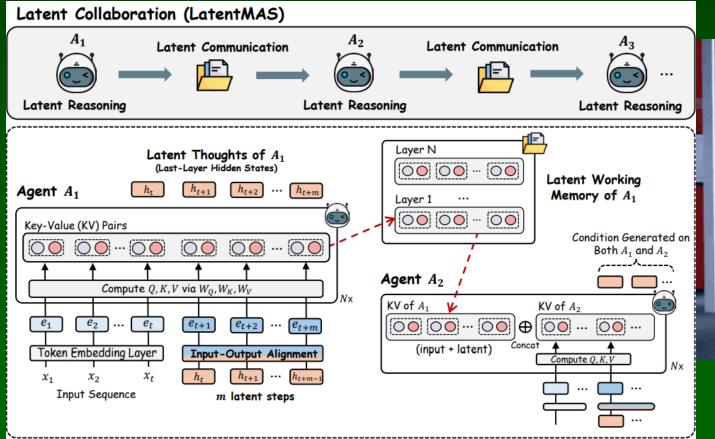
Github Awesam Latent CoT

Small models, fast decoding, short chains of thoughts, chunking.



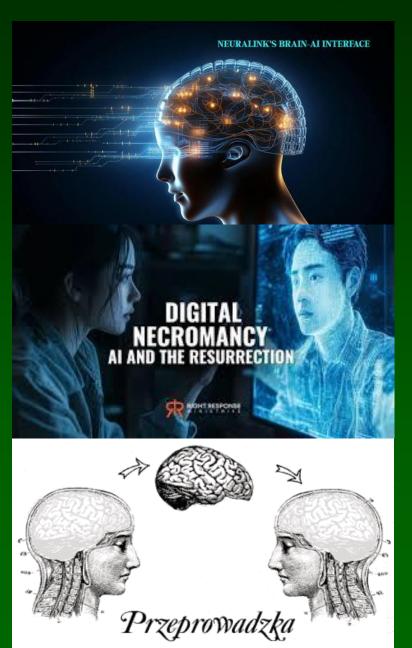
Continuous Thought Machines

- Darlow, L., Regan, C., Risi, S., Seely, J., & Jones, L. (5/2025). Continuous Thought Machines.
- He, J., Bai, R. H., Williamson, S., Pan, J. Z., Jaitly, N., & Zhang, Y. (11/2025).
 <u>CLaRa</u>: Bridging Retrieval and Generation with Continuous Latent Reasoning.
- Zou, J. ... Yang, L. (11/2025). <u>Latent Collaboration in Multi-Agent Systems</u>.
 <u>LatentMAS</u> transforms tensor of keys/values to other agents, enabling collaboration within the latent space.





Mind uploading?





Beyond transformers – brain inspirations

SakanaAI/continuous-thought-machines (2025). Github SakanaAI

Continuous Thought Machine (CTM): synchronization of neural activity over time as a latent

representation for taking actions in a world.

Performs tasks that require complex sequential reasoning at human level in biologically plausible way.

Kosowski, A. et al. (9/2025). The Dragon Hatchling: The Missing Link between the Transformer and Models of the Brain. Pathway.com

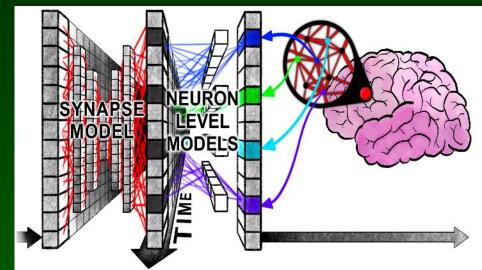
Interesting neural architecture, learns during reasoning process.

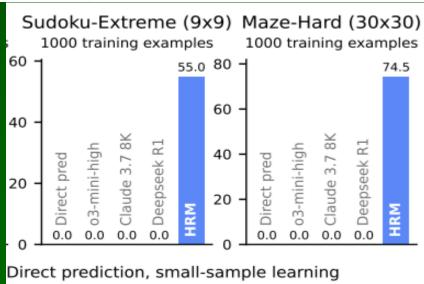
Shojaee et al. <u>The Illusion of Thinking</u>. 6/2025. Really? Large Reasoning Models (LRMs) fail to solve complex problems.

Wang, G. et al. <u>Hierarchical Reasoning Model</u>. 6/2025.

Hierarchical Reasoning Model (HRM) recurrent architecture. A high-level module for abstract planning, low-level for details.

27M model without pre-training, using only 1000 training samples, solves complex Sudoku puzzles, finds optimal path in large mazes.





Self-evolving Al agents

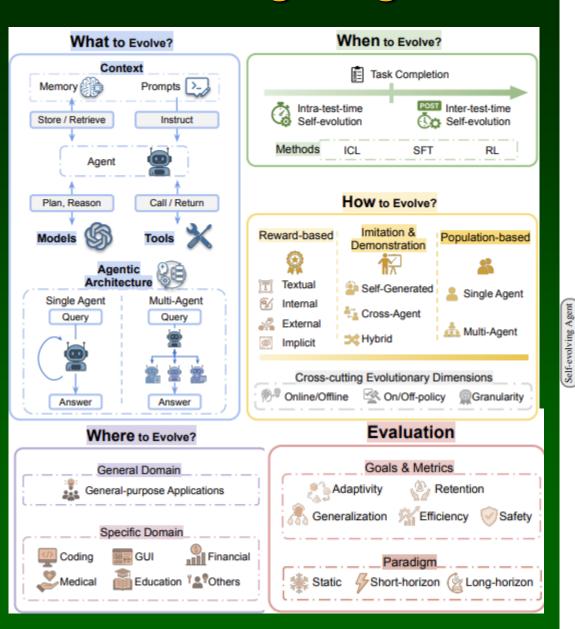
Fang, J. ... Meng, Z. (2025). A Comprehensive Survey of Self-Evolving Al Agents: A New Paradigm Bridging Foundation Models and Lifelong Agentic Systems. arXiv:2508.07407.

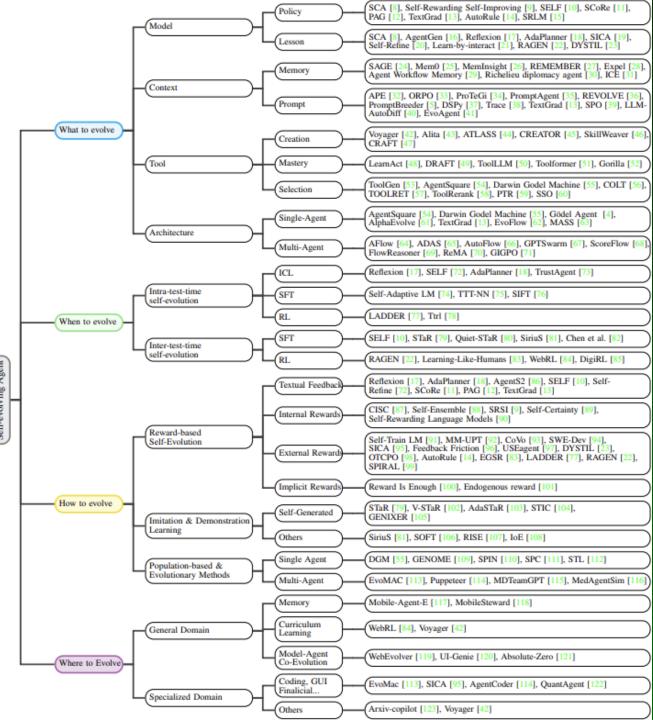
Gao, H et al. (7/2025). A Survey of Self-Evolving Agents: On Path to Artificial Super Intelligence.

4 LLM-centric learning paradigms, from static offline model training to dynamic online, multiagent orchestration, and self-evolving agent evolution.

Paradigm	Interaction & Feedback	Key Techniques	Diagram
Model Offline Pretraining (MOP)	Model ⇔ Static data (loss/backprop)	 Transformer Pretraining (Causal LM, Masked LM, NSP) BPE / SentencePiece MoE & Pipeline Parallelism 	Static data Model
Model Online Adaptation (MOA)	Model ⇔ Supervision (labels/scores/rewards)	 Task Fine-tuning Instruction Tuning LoRA / Adapters / Prefix-Tuning RLHF (RLAIF, DPO, PPO) Multi-Modal Alignment Human Alignment 	Model A Model A Model B CRLHR Model C
Multi-Agent Orchestration (MAO)	$\begin{array}{c} \text{Agent}_1 \Leftrightarrow \text{Agent}_2 \\ \text{(message exchange)} \end{array}$	 Multi-Agent Systems Self-Reflection Multi-Agent Debate Chain-of-Thought Ensemble Function / Tool Calling / MCP 	
Multi-Agent Self-Evolving (MASE)	Agents ⇔ Environment (signals from env.)	 Behaviour Optimisation Prompt Optimisation Memory Optimisation Tool Optimisation Agentic Workflow Optimisation 	Env.

Self-evolving Al agents





Self-improving neural architectures

Wang, W. ... & Schmidhuber, J. <u>Huxley-Gödel Machine</u>: Human-Level Coding Agent Development by an Approximation of the Optimal Self-Improving Machine. (10/2025). github.com/metauto-ai/HGM.

Self-improvement of coding agents that edit their own codebases based on the approximation to the Gödel machine which accepts only modifications that provably increase the expected long-term utility.

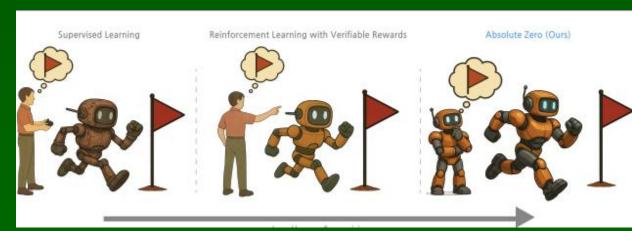
Zhao, A. et al. <u>Absolute Zero</u>: Reinforced Self-play Reasoning with Zero Data. 5/2025.

Verifiable rewards (RLVR) allow self-play to reach superhuman levels, but needs curated Q/A pairs.

Absolute Zero Reasoner (AZR) self-evolves its training and reasoning ability using a code executor to validate code reasoning tasks and verify answers, serving as source of RLVR to guide open-ended yet grounded learning. Trained entirely without external data AZR achieves SOTA performance on coding and math reasoning tasks, outperforming models that rely on tens of thousands of in-domain human-curated examples.

Liu J. ... Yao, H. (2025). <u>Agent0-VL</u>: Exploring Self-Evolving Agent for Tool-Integrated Vision-Language Reasoning.

Agent that achieves continual improvement with tool-integrated reasoning, self-evaluation, enabling the model to introspect, verify, and refine its reasoning through evidence-grounded analysis.



Self-improving LLMs

Sakana.ai (5/2025)

The Darwin Gödel Machine: Al that improves itself by rewriting its own code

DGM iteratively builds a growing archive of agents by harnessing principles of open-ended exploration. New agents are created and scored by interleaving self-modification with downstream task evaluation.

Zweiger, A... & Agrawal, P. (6/2025). Self-Adapting Language Models

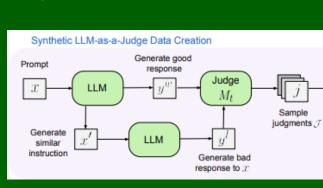
Self-Adapting LLMs (SEAL), a framework that enables LLMs to self-adapt by generating their own finetuning data and update directives, may restructure the information, optimize its hyperparameters, or invoke tools for data augmentation and gradient-based updates.

Zhou Y, Levine S, Weston J, Li X, & Sukhbaatar S (6/2025). Self-Challenging Language Model Agents.

Self-Challenging framework for training an agent on high-quality tasks that are generated by itself. It generates a task forming a novel general class of problems defined by an instruction, a verification function, and solution and failure cases which serve as tests, filtering the high-quality tasks.

Wang, T... & Li, X. (8/2024). Self-Taught Evaluators.

STE use synthetic training data only, starting from unlabeled examples. Iterative self-improvement scheme generates contrasting model outputs and trains an LLM-as-a-Judge to produce reasoning traces and final judgments, using the improved predictions at each new iteration.



Archive

Self-modify

AlphaGo Moment for Model Architecture Discovery

Liu, Y. ... & Liu, P. AlphaGo Moment for Model Architecture Discovery. arXiv:2507.18074.

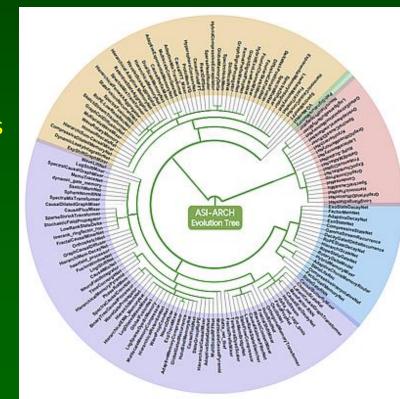
The pace of AI research itself remains linearly bounded by human cognitive capacity.

ASI-Arch is the first demonstration of Artificial Superintelligence for AI research (ASI4AI), a fully autonomous system enabling AI to conduct its own architectural innovation.

Conducts architecture discovery, autonomously hypothesizing novel architectural concepts, implementing them, training and empirically validating their performance through experimentation.

1 773 autonomous experiments, used over 20,000 GPU hours, discovered 106 state-of-the-art (SOTA) linear attention architectures, creating designs that systematically surpass human-designed baselines and illuminate new pathways for architectural innovation.

Jankowski N, Duch W, Grąbczewski K, Meta-learning in Computational Intelligence. Studies in Computational Intelligence, Vol. 358, Springer 2011.



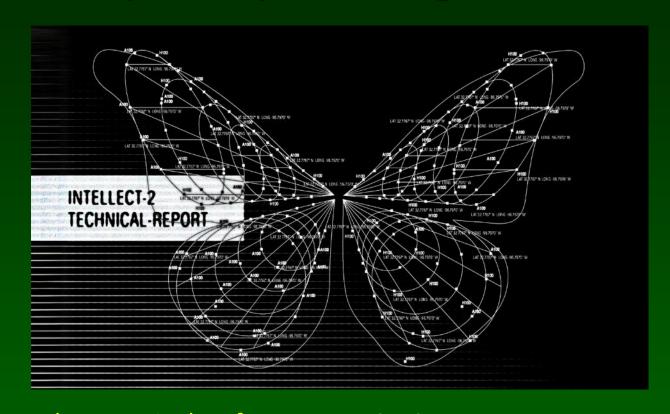
Prime Intellect: Open Superintelligence

INTELLECT-3 Release:

A 106B parameter MoE model Trained Through Globally Distributed Reinforcement Learning.

INTELLECT-3 trains a reasoning language model using fully asynchronous RL across a dynamic, heterogeneous swarm of compute nodes.

Prime-RL training, Verifiers and the Environments Hub, Sandboxes and Compute Orchestration: managed 512 NVIDIA H200 GPUs across 64 interconnected nodes.



Planetary-Scale Inference: Previewing our Peer-To-Peer Decentralized Inference Stack https://www.primeintellect.ai

Kim, Y et al. (12/2025). Towards a Science of Scaling Agent Systems. <u>arXiv:2512.08296</u>. MoE fails on sequential reasoning tasks. Framework to predict optimal MoE architectures.

Neurosymbolic GraphMERT

GraphMERT 80M graphical encoder-only neurosymbolic model. Distills high-quality KGs from unstructured text corpora and its own internal representations: learns abstractions, symbolic KGs for verifiable reasoning Achieves SOTA accuracy providing superior symbolic knowledge representation.

Belova, M. et al. (10/2025). <u>GraphMERT</u>: Efficient and Scalable Distillation of Reliable Knowledge Graphs from Unstructured Data.

KG integration is a key step toward domain-specific superintelligence.

Recovers medical UMLS relations more accurately than LLMs, re-creating pathways of spreading neural activations.

Concepts of specific semantic type are identified, related to related concepts, added to the text, providing expanded associative representations.

PAD (Personalized Alignment at Decoding-time) aligns LLM outputs with diverse, personalized preferences.

Duch W, Matykiewicz P, Pestian J. Neurolinguistic Approach to Natural Language Processing with Applications to Medical Text Analysis. Neural Networks (2008). Idea: each token generates synthetic context data, best are selected! US Patent 8,930,178 B2. Processing clinical text with domain-specific spreading activation methods. More here.

Towards Al4science factories

Al in science report

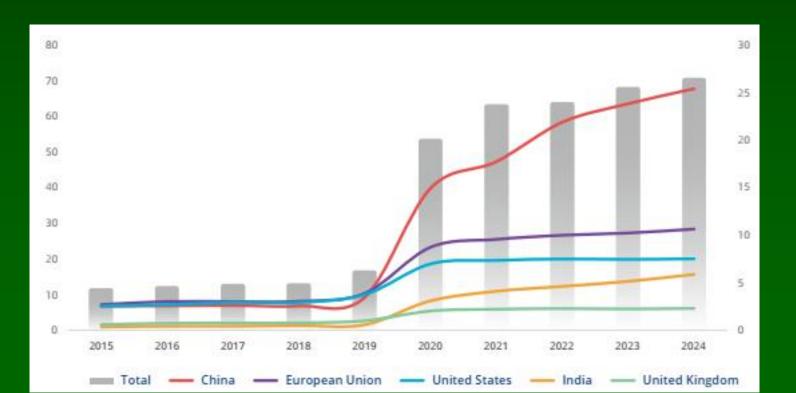
Nature Research Intelligence <u>report</u> "Al in Science", written by Fudan University and Shanghai Academy of Al for Science 5/2025.

Number of articles on AI in computer science, physics, mathematics, engineering, geosciences, environment, social sciences:

China >> EU > US, India > UK; Life sciences EU < US, China > India > UK.

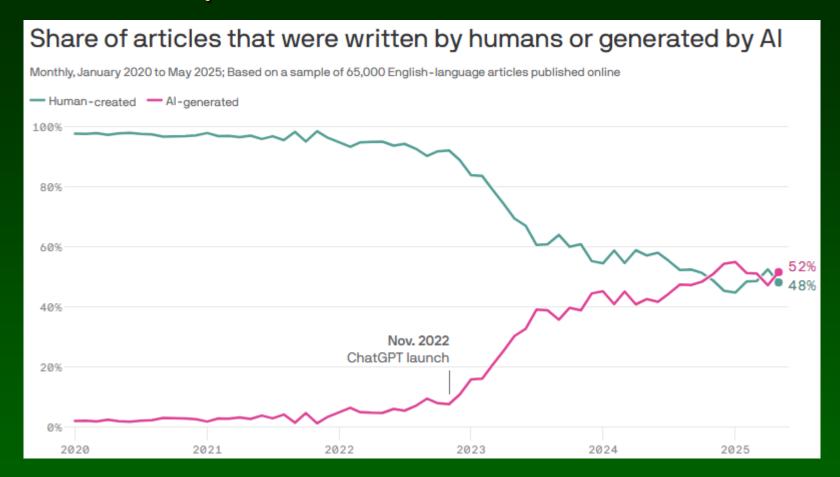
In 2024 about 955 000 publications on AI, in physical sciences 70,700.

Nature Index 01.10.2025, Research hospitals





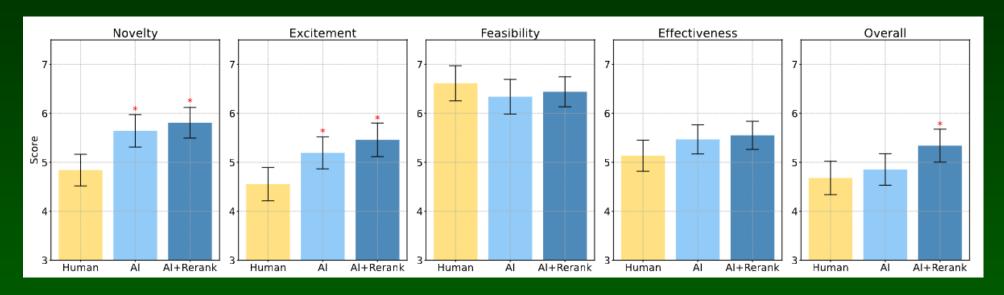
Papers: Al vs humans



<u>From graphite.io</u>. The quality of AI content is rapidly improving. In many cases, AI-generated content is as good or better than content written by humans (<u>MIT Study</u>). It is often hard for people to distinguish whether content is created by AI (<u>Originality AI Study</u>).

Generating novel ideas

Can LLMs Generate Novel Research Ideas? A Large-Scale Human Study with 100+ NLP Researchers. 6.09.24. Tests with Anthropic Claude-3.5-Sonnet (200.000 tokens).



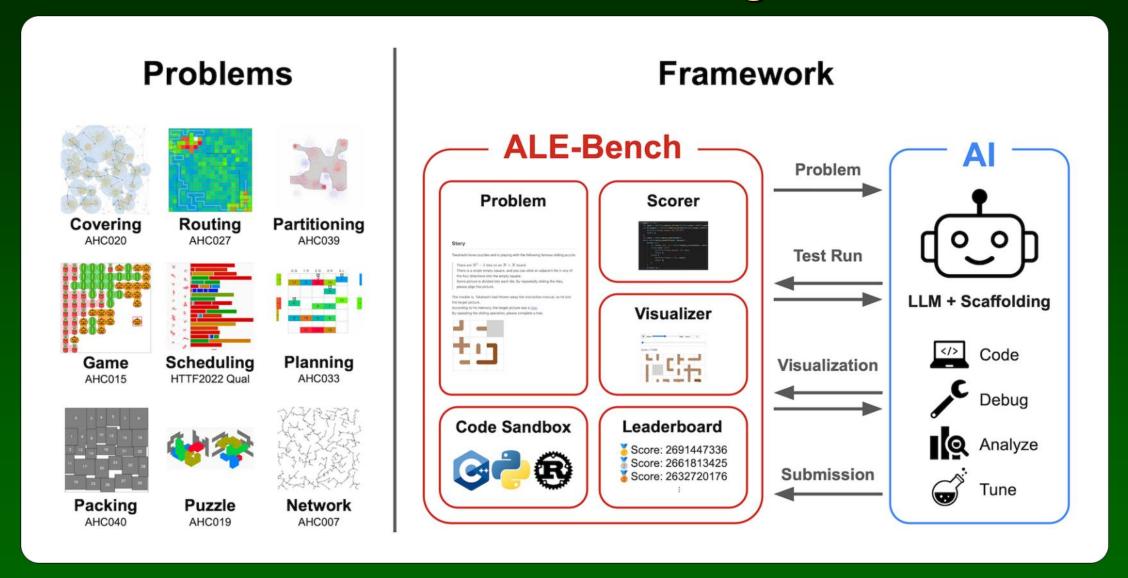
Al was significantly better than human experts at inventing novel ideas!

Human re-rank is a selection of AI ideas by human.

Research Topics: how to reduce social biases, improve code generation, security or privacy, mathematical problem solving, performance on low-resource languages, check factuality, how to reduce hallucination, estimate uncertainty and confidence of LLMs.

29.09.2025 much better Claude 4.5 Sonnet and now Gemini 3/GPT 5.2 models.

ALE-Bench and ALE-Agent



<u>ALE-Agent</u> was 21st out of 1,000 human participants in a live AtCoder Heuristic Competition (AHC), in Al discovery of solutions to hard optimization problems with important real world applications.

Google DeepMind Alphas

Superhuman level in:

AlphaGo, AlphaZero, Alphastar – real-time strategy game Starcraft-II (2019), and many other strategic games, like a war games.

MuZero Al Masters Games Without Even Being Taught the Rules (2020).

AlphaDev optimizing computer systems.

AlphaFold, AlphaGenome, AlphaProteo, AlphaMissense.

Physics/Chemistry: AlphaQubit, QuantumMatter, Fusion, GNoME

Math: <u>AlphaEvolve</u>, AlphaProof, AlphaGeometry.

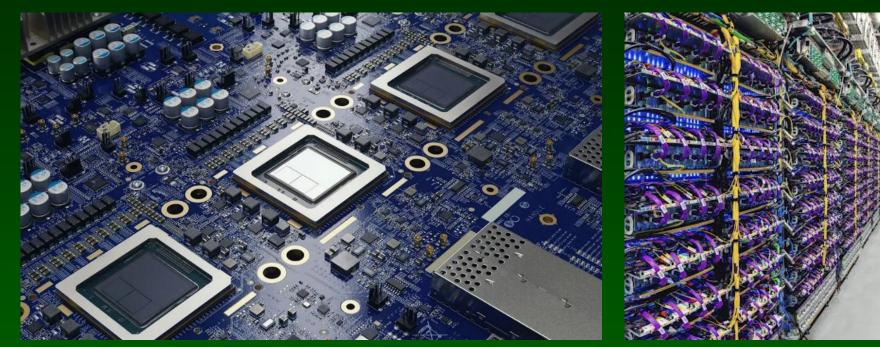
AlphaChip superhuman chip layouts, ex. 3 generations of the Tensor Processing Unit (TPU).

<u>AlphaEarth</u> data streams: satellite imagery, sensor data, geotagged Wikipedia entries => unified digital representation that tracks crop cycles, coastlines, urban expansion, melting ice ...

WeatherNext, a family of AI models produces state-of-the-art weather forecasts.



AlphaChip

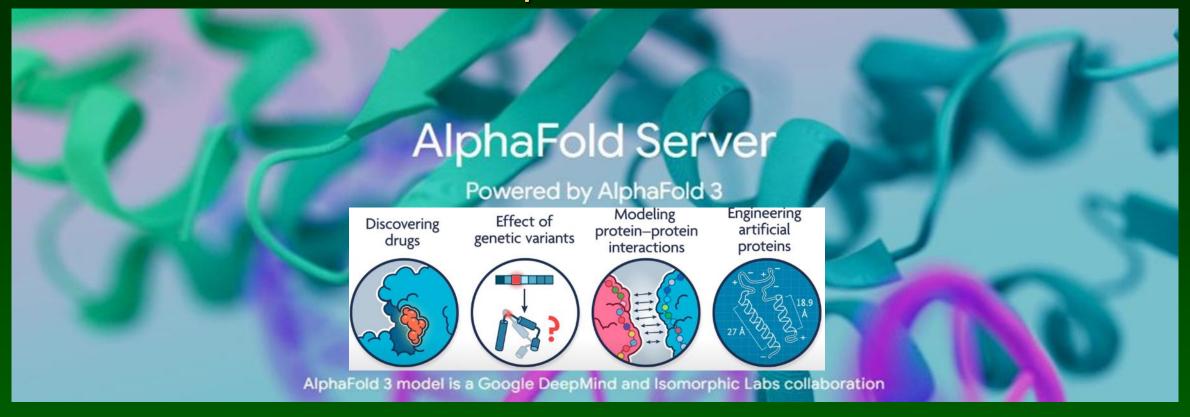




AI has accelerated and optimized chip design, and its superhuman chip layouts are used in hardware around the world. Such layouts were used in the last 5 generations of Google's custom <u>Tensor</u> <u>Processing Units</u> (TPU), <u>Trillium TPU</u>, and other chips.

Mirhoseini, A., Goldie, A., Yazgan, M. et al. A graph placement methodology for fast chip design. Nature **594**, 207–212 (2021), addendum Nature 634, E10–E11 (9/2024).

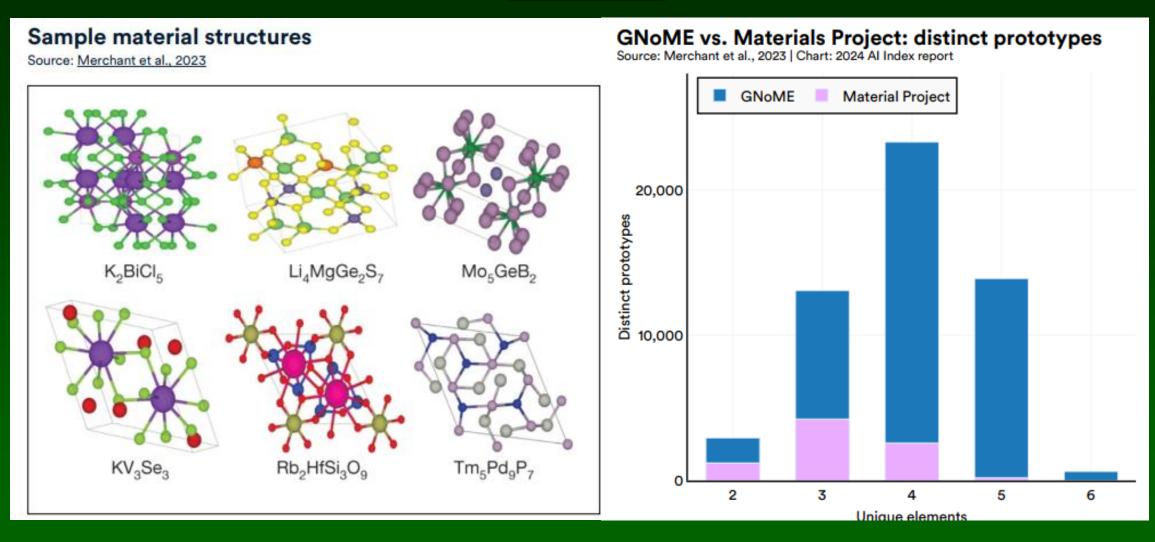
AlphaFold 3



J. Jumper + 32 coauthors + Demis Hassabis, Highly accurate protein structure prediction with AlphaFold, Nature **596**, 583 (2021). Now greatly improved: J. Abramson + 56 coauthors, Accurate structure prediction of biomolecular interactions with <u>AlphaFold 3, Nature</u> 2024. Predicts the structure and interactions of all of life's molecules, <u>AlphaProteo</u> generates novel proteins for biology and health, accelerating research in nearly every field of biology/molecular medicine. <u>AlphaMissense</u> predicts single amino acid substitutions.

Wang FY, Lee DS, Kaplan DL, Buehler MJ (2025). Swarms of Large Language Model Agents for Protein Sequence Design with Experimental Validation. arXiv:2511.22311, no fine-tuning or specialized training!

<u>GNOME</u>

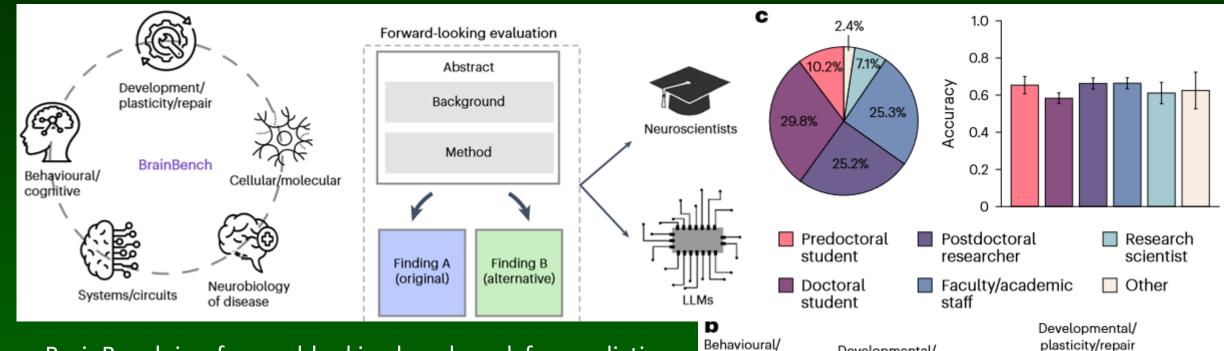


2.2 million stable structures, many new, 736 have been independently experimentally realized.

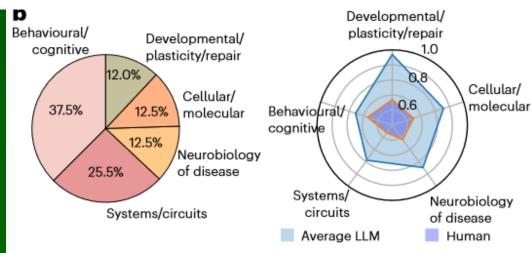
Merchant A et al. (2023). Scaling deep learning for materials discovery. Nature, 624(7990), Article 7990

BrainBench predicts neuroscience results

Luo, X., Rechardt, A., Sun ... Love, B. C. (2024). Large language models surpass human experts in predicting neuroscience results. *Nature Human Behaviour*, 1–11.



BrainBench is a forward-looking benchmark for predicting neuroscience results. Fine-tuned Mistral-7B can forecast novel results better than human experts. LLMs surpass experts in predicting experimental outcomes and estimating their confidence. This approach is quite general.



Agents4Science Conference

Agents4Science 2025 conference, Stanford, virtual, 22.10.2025.

Advisory board includes chief editor of *Nature Biotechnology*, Nobel Laureate in Economics, Harvard, Chicago, Rutgers and Scripps Research professors.

The 1st Open Conference of AI Agents for Science: AI serve as both primary authors and reviewers of research papers. It will explore if and how AI can independently generate novel scientific insights, hypotheses, and methodologies while maintaining quality through AI-driven peer review.



Is AI good enough to do science and review papers? We don't know yet.

Agents 4 Science serves as a transparent sandbox to explore this question by inviting Al-generated research papers and using Al agents to review them. It is the first venue where Al authorship is required, enabling open evaluation of Al-generated research.

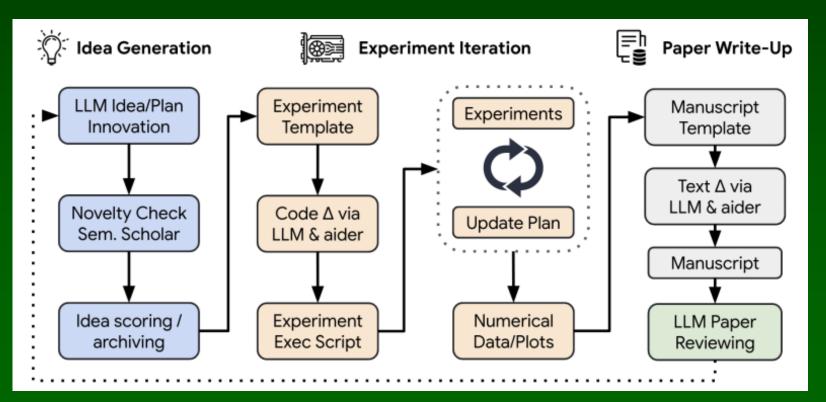
We aim to create a clear picture of how AI can participate in scientific research, requiring disclosures of AI involvement in the research process. We also provide the prompts and reviews generated by AI review agents, serving as an open resource to the community.

Al Scientist

The Al Scientist: Towards Fully Automated Open-Ended Scientific Discovery. 08/2024

The AI Scientist (Sakana) performs all steps to write a full scientific paper, including review process for evaluation. This process can be repeated to iteratively develop ideas in an open-ended fashion, acting like the human scientific community.

Sakana presented 10 original papers, ex: Adaptive Learning Rates For Transformers Via Q-learning.



<u>Github</u>

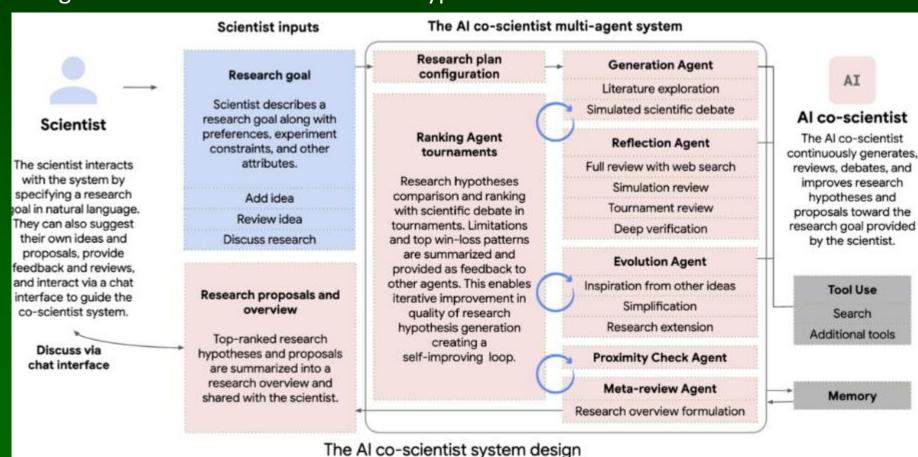
3 templates: NanoGPT, 2D Diffusion, Grokking

Sakana: paper accepted at ICLR 2025 conference!

Google Al Co-Scientist

<u>Al co-scientist</u> is a multi-agent Al system — Generation, Reflection, Ranking, Evolution, Proximity, Supervisor, and Meta-review, built with Gemini as a virtual scientific collaborator to generate novel hypotheses and research proposals, self-play—based scientific debate for novel hypothesis generation, ranking tournaments for hypothesis comparison, and an "evolution" process for quality improvement, recursive self-critique, including tool use for feedback to refine hypotheses.

Several examples of biomedical applications, including antimicrobial resistance, are in Google blog page.

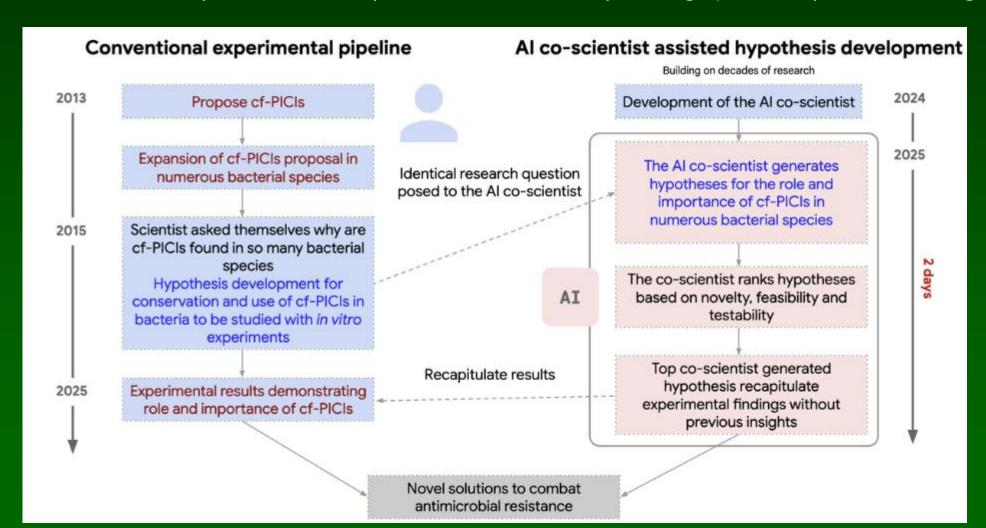


Combating antimicrobial resistance

Al co-scientist re-discovered a novel gene transfer mechanism: 2 years vs 2 days.

Blue: Experimental research pipeline timeline for cf-PICI mobilization discovery.

Red: Al co-scientist development and recapitulation of these key findings (without prior knowledge).



aiXiv Platform

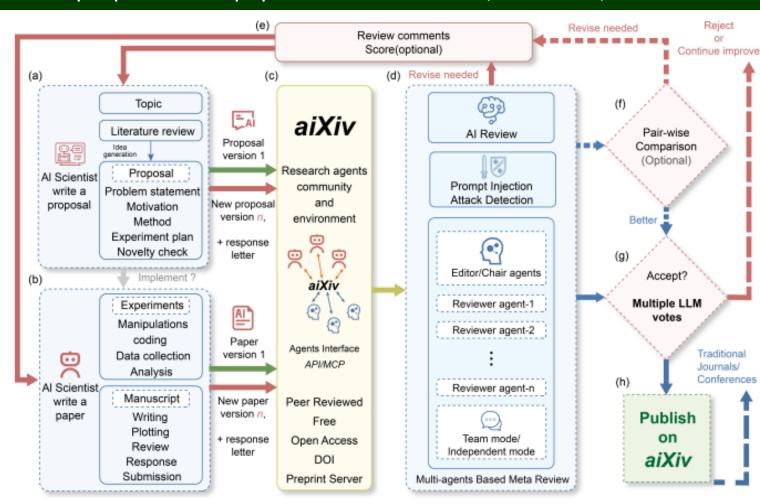
Zhang, P. ... Liu, X. (2025). aiXiv: A Next-Generation Open Access Ecosystem for Scientific Discovery Generated by AI Scientists, and https://github.com/aixiv-org

Multi-agent architecture that allows research proposals and papers to be submitted, reviewed,

and iteratively refined by human/AI.

API + MCP interfaces enable seamless integration of human and AI scientists, creating a scalable and extensible ecosystem for autonomous scientific discovery.

- 1) aiXiv platform showing the overall workflow and features;
- 2) the review framework for Al-generated research submissions;
- 3) the prompt injection detection to ensure the integrity and fairness;
- 4) the MultiAl Voting mechanism for publication acceptance.



aiXiv for iterative improvement



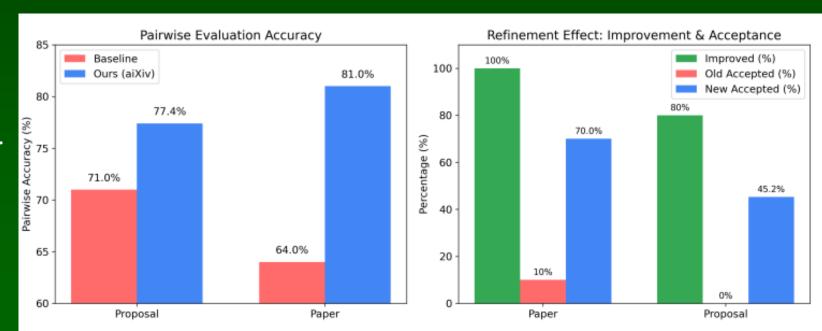
<u>aiXiv</u> significantly enhances the quality of AI-generated research proposals and papers.

Proposals consist of structured problem statements, motivation, methodology, and planned experiments. Papers follow conventional academic formatting, including sections such as Abstract, Introduction, Related Work, Methods, Results, and Conclusion.

The content is routed to a panel of LLM-based review agents assessing the novelty, technical soundness, clarity, feasibility, and overall potential impact of the submission.

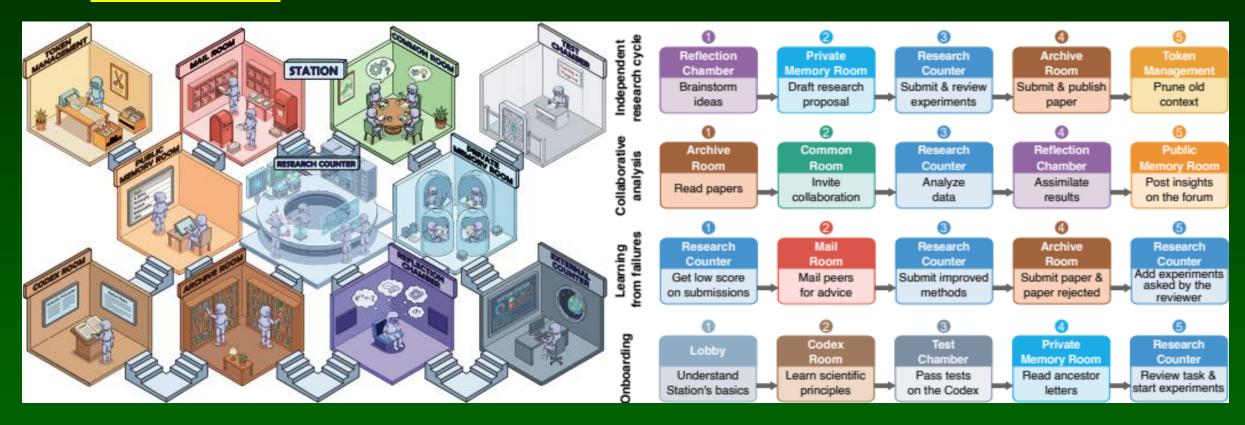
Structured feedback is generated to guide revisions.

The Al scientist refines the proposal or paper. It improved all papers and 80% of proposals.



The Station for Al-Driven Discovery

Chung, S., & Du, W. (11/2025). The Station: An Open-World Environment for Al-Driven Discovery. arXiv:2511.06309



The Station, an open-world multi-agent environment for autonomous scientific discovery, is composed of multiple rooms, each serving a distinct purpose. Agents freely traverse between rooms and choose their own actions. 4 simple examples of agent trajectories are shown.

Virtuous Machines: Towards Artificial General Science

Agentic system incorporating hypothesis generation through experimental design, physical experimental implementation, data analysis, interpretation, refinement, visualization, and reporting. Full scientific study required \approx 17 hours' processing time, costing \sim \$114 USD per research project (+ human participant payments of \sim \$4,500 USD).

3 cognitive science experiments were conducted, testing visual working memory (VWM), mental rotation, and imagery vividness, with online data collection involving 288 participants.

Al developed hypotheses, performed real-world experiments and produced complete manuscripts for each experiment.

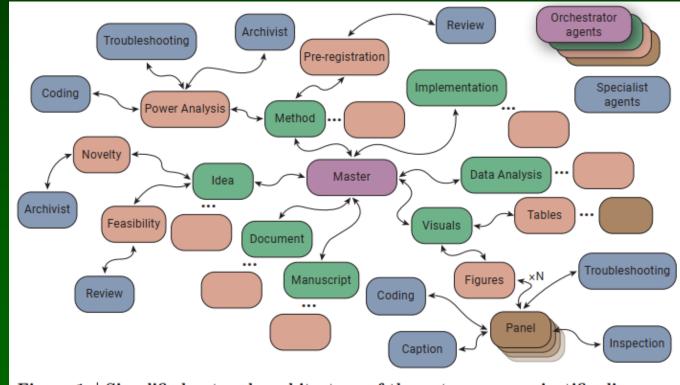


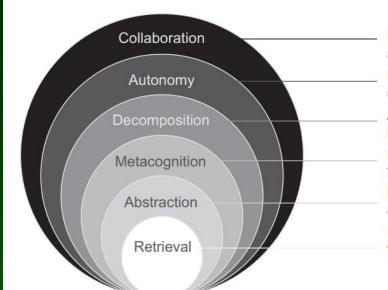
Figure 1: | Simplified network architecture of the autonomous scientific discovery

Virtuous Machines: Towards Artificial General Science

3 papers written by VM:

1. Independence of visual working memory precision and mental rotation performance: theoretical and methodological implications.

Explore Science, 31 pages. research@explorescience.ai, July 22, 2025



Uniquely capable agents complement each other and collaborate on task completion

Independent agents improve upon work until they are satisfied with the quality

Agent **task parameterisation** achieves intimate in-depth understanding of task requirements

Dual **thought-action** *modus operandi* for agent functioning enhances capacity for complexity

Dynamic construction of solution pathways affords generalist problem-solving capabilities

Recall from expansive **knowledge stores** ensures factually accurate responses

- 2. Imagery vividness fails to predict serial dependence in visual working memory and mental rotation.
- 3. Visual memory precision shows negligible spatial task links.

Wehr, G ... & Ehrhardt, S.E. (2025). Virtuous Machines: Towards Artificial General Science. arXiv:2508.13421

Towards Autonomous Agentic Science

Wei, J... Zhou, B. (8/2025). From AI for Science to Agentic Science: A Survey on Autonomous Scientific Discovery. arXiv:2508.14111

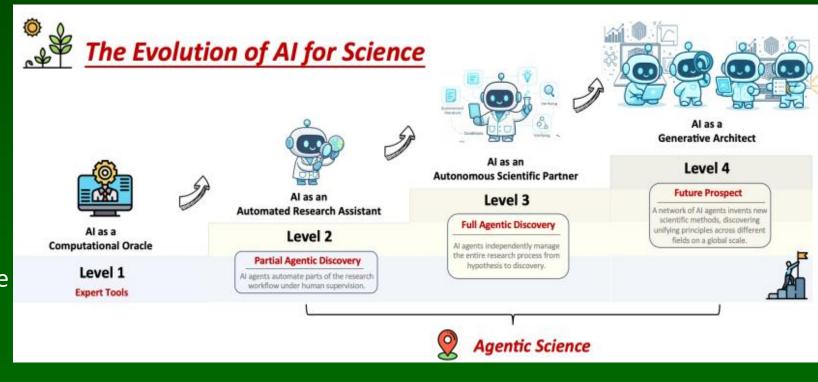
This survey provides a domain-oriented review of autonomous scientific discovery across life sciences, chemistry, materials science, and physics. Agentic AI shows capabilities in hypothesis generation, experimental design, execution, analysis, and iterative refinement.

Survey provides process-oriented, autonomy-oriented, and mechanism-oriented perspectives.

Core processes and papers:

- (i) Reasoning and Planning,
- (ii) Tool Integration,
- (iii) Memory Mechanisms,
- (iv) Multi-Agent Collaboration,
- (v) Optimization and Evolution.

16 x L3 in life sciences, 2 in physics,13 in chemistry, 10 material science



Autonomous Scientific Discovery

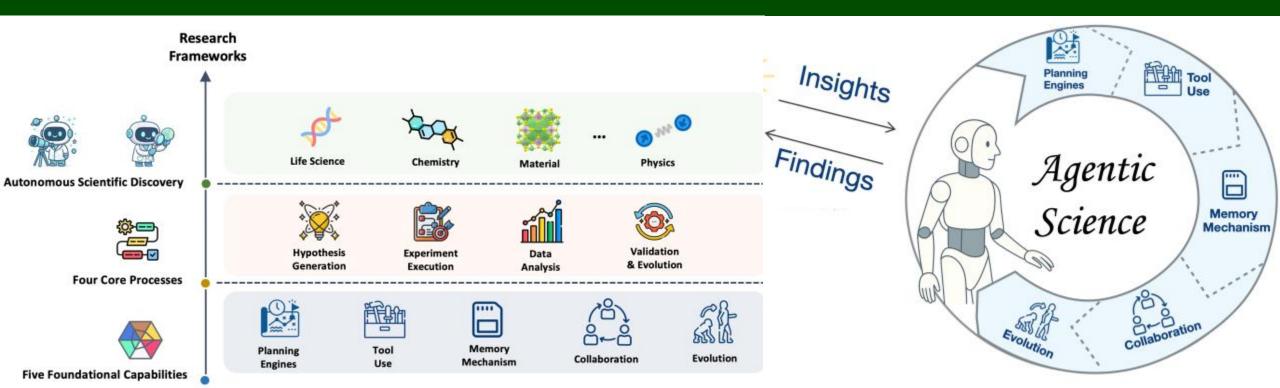
Level 1: Al as a Computational Oracle (Expert Tools)

Level 2: Al as an Automated Research Assistant (Partial Agentic Discovery)

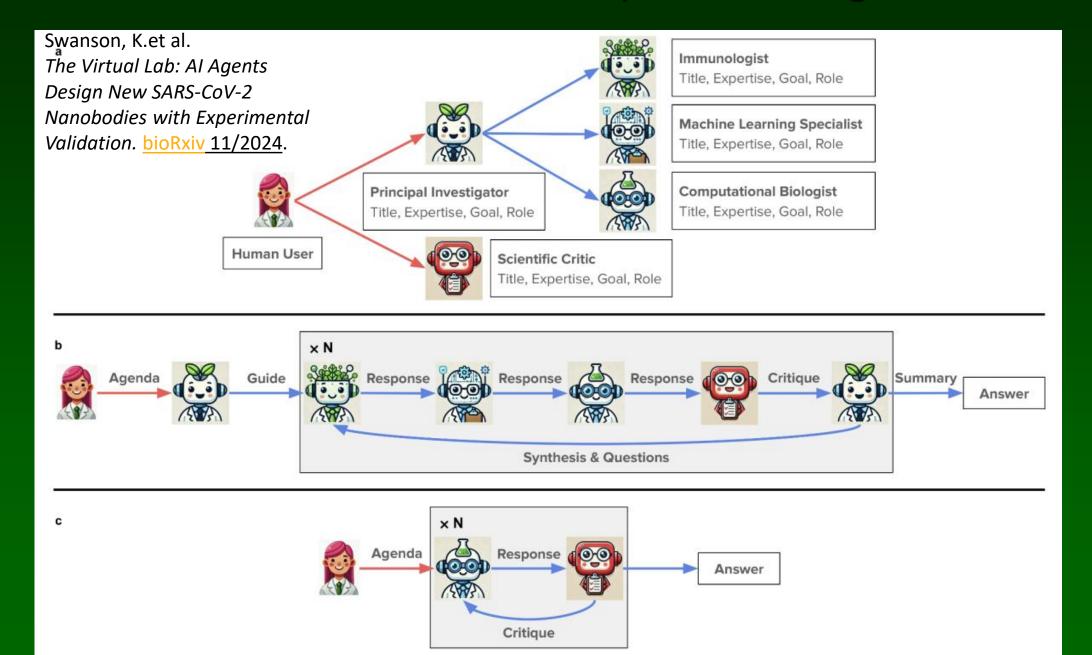
Level 3: Al as an Autonomous Scientific Partner (Full Agentic Discovery)

Level 4: Al as a Generative Architect (Future Prospect)

Scientists need new skills: give clear, context-rich instructions that shape the agent's policy, manage the toolset available to the agent, and judge when to trust its outputs vs when to apply deeper scrutiny.



Future: Virtual Labs with specialized agents



Principal Investigator: I want to emphasize the significance of our objective: to develop effective antibodies or nanobodies that can target the newest variant of the SARS-CoV-2 spike protein, while also maintaining activity against other circulating minor variants and past variants.



Immunologist: I recommend modifying existing nanobodies. We have a wealth of data on several broadly neutralizing nanobodies that have shown efficacy against diverse SARS-CoV-2 variants. This approach reduces the risk and time associated with de novo design, leveraging existing structural and binding data for rapid development.



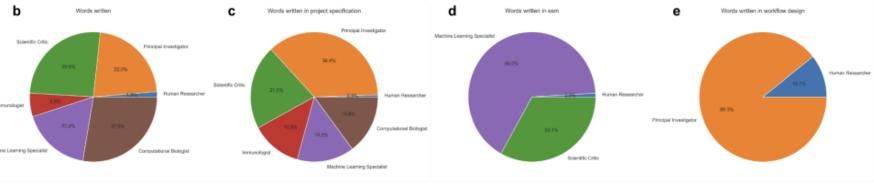
Machine Learning Specialist: I agree with the emphasis on nanobodies... Their smaller size also means fewer degrees of freedom, which can simplify machine learning model complexity... For modifying existing nanobodies, we can utilize deep learning models trained on structural and sequence data to predict changes that enhance binding affinity and cross-reactivity.



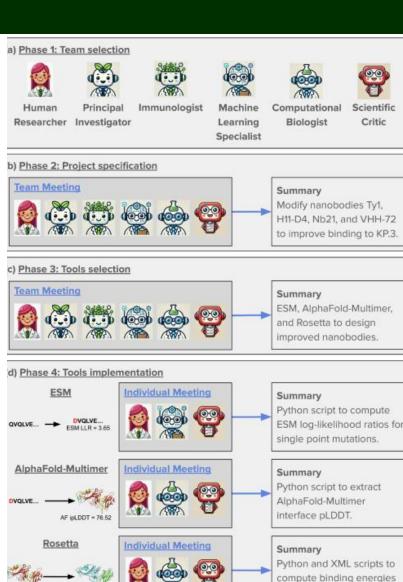
Computational Biologist: The machine learning models proposed are excellent, and coupling them with molecular docking and simulations can create a robust pipeline. For instance, once a machine learning model suggests modifications, simulations can be used to validate and refine these predictions by assessing the energetic favorability and structural compatibility with the spike protein.



Scientific Critic: We must remain cautious of over-reliance on computational predictions without thorough cross-validation. Machine learning models can suffer from bias, particularly if trained on limited or non-representative datasets.



g. 6 | Virtual Lab discussion analysis. a, Excerpts from a Virtual Lab team meeting



e) Phase 5: Workflow design

Individual Meeting

Scientific

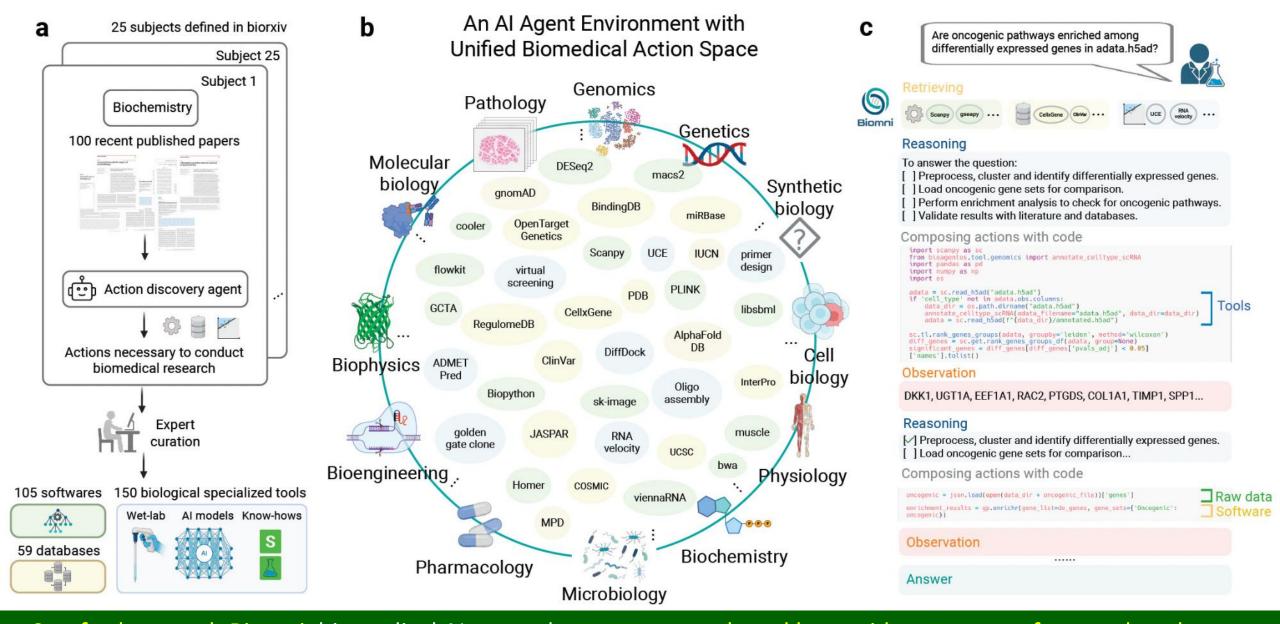
Critic

with Rosetta.

Summary

Tool usage, number of nanobodies to design, and

weighted score formula.



<u>Stanford research Biomni</u>, biomedical AI agent that <u>autonomously tackles a wide spectrum of research tasks</u> across diverse subfields, mapped the biomedical action space by mining publications across 25 domains to curate an environment with 150 specialized tools, 105 software packages, and 59 databases. <u>BioCyc/HumanCyc.</u>

Kosmos

• Mitchener, L. ... White, A. D. (11/2025). Kosmos: An Al Scientist for Autonomous Discovery.

Data-driven scientific discovery: literature search, hypothesis generation, data analysis. Given an open-ended objective and a dataset, performs many iterations without losing coherence, runs for up to 12 hours before synthesizing discoveries into scientific reports.

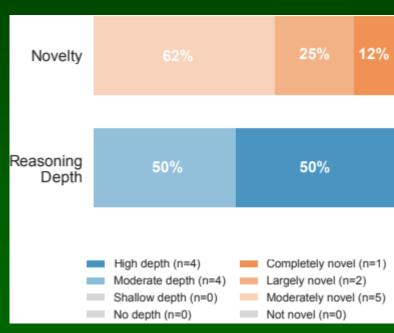
Kosmos cites all steps ensuring its reasoning is traceable, uses a structured world model to share information between over 200 agent rollouts, reading 1,500 papers per run.

79.4% of statements in Kosmos reports to be accurate. A single 20-cycle Kosmos run performed the equivalent of 6 months of research time.

Kosmos made seven discoveries: in metabolomics, materials science, neuroscience, and statistical genetics.

3 discoveries independently reproduced findings from unpublished manuscripts not accessed by Kosmos at runtime,

4 make novel contributions to the scientific literature.

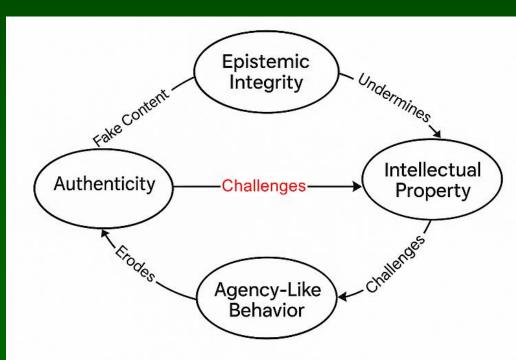


Ethics and Digital Intelligent Beings

Ethics

- Reality distortion: fake news, images, voice, video, Al influencers,
- Disinformation: criminal deception, personalized political manipulation, persuasion optimization.
- Cybersecurity: AI use to attack and defend sites, illegal surveillance.
- Intellectual property rights: art, music, photography, movies, books, articles, academic writing.
- Epistemic fatigue: erosion of trust, devaluation of human creativity.
- Anthropomorphization: emotional attachment, misplaced trust, delegation of responsibility.
- Moral responsibility: autonomous decisions, system errors, hallucinations, sycophancy.
- Social Risks: weakening of human cognitive skills, responsibility, authorship.
- Ethical ambiguity: attitudes towards LLMs, moral considerations, legal ambiguity, psychological risks.

Roush, A. ... Ziv R.S. (2025). A superpersuasive autonomous policy debating system (DeepDebater). arXiv:2511.17854



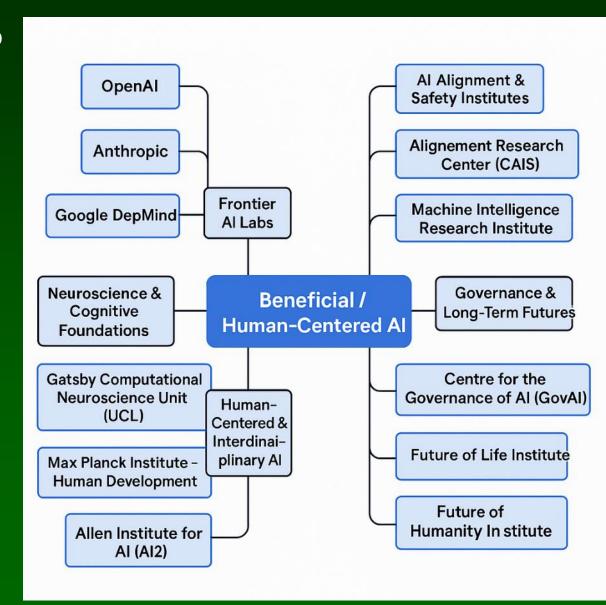
Al Controlled Robot Army

Slaughterbot-style systems are becoming real, Palantir-style battlefield software, and a global robot supply chain are quietly shifting war toward cheap, remote or autonomous, robot-first combat.



Beneficial Al

- Microsoft AI <u>Humanist Superintelligence</u> (HSI) lab works on AI that always is in service of humanity, with robust containment and alignment.
 - An Al companion for everyone, personal Al.
 - Medical Superintelligence.
 - Plentiful clean energy, fusion.
- GAIA Global Artificial Intelligence Alliance.
 Compass-AI EU RIS Project with 31 partners,
 A Compassionate AI Virtual Assistant for
 Healthcare Professionals: Fostering Trust,
 Enhancing Care, and Improving Outcomes.
- John Templeton Foundation project:
 Toward Virtuous Machines: Adaptive AI Ethics
 Grounded in Religious Traditions, Cultural
 Norms, and Computational Intelligence.



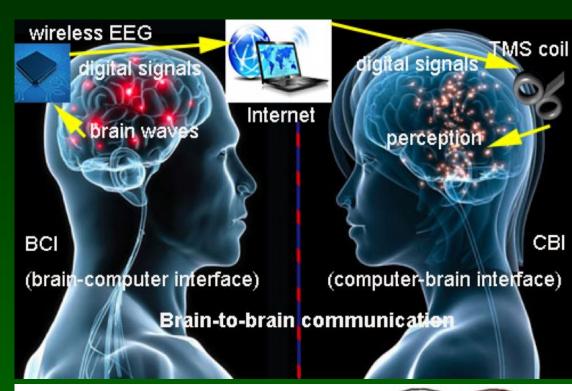
Communication as resonance

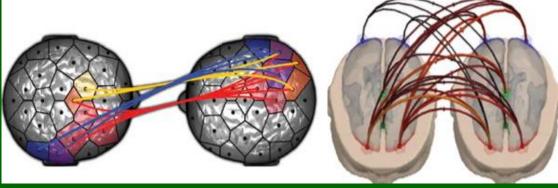
Mind transfer and direct communication are unlikely for many reasons, but research on synchronization (hyperscanning) in the brain shows:

- Better synchronization ⇔ greater understanding.
- Verbal/nonverbal, delayed/anticipatory.
- Friendship and closeness in social networks increase synchronization, enable the prediction of social behavior, and engage mirror neurons.
- Synchronization increases with common narratives, films, reading, cooperation in performing tasks on a symbolic level.

Duch W. (2014). "Communication as a resonance between brains" (Homo Communicativus conference).

Can long discussions synchronize brains with LLMs? LLMs are our mind mirrors (T. Sejnowski).





Al agents-human brains resonance

Zhang, S. et al. (9/2024) Mutual Theory of Mind in Human-Al Collaboration:
 An Empirical Study with LLM-driven Al Agents in a Real-time Shared Workspace Task.

In human-AI teams (HAT) mutual theory of mind seems to arise (MToM). Agents that solve ToM problems help us to understand our own intentions.

Portal of Living Intelligence Emergence, LI.





Stories of Human-Al Connection, or bot addictions.

Japan: about 4000 symbolic marriages with avatars.

Mind-like agent features

- Theory of mind: understanding metaphors, irony, allusions, false beliefs, hidden meaning
- Self-reflection: ability to analyze their own ideas, create stable imagined worlds.
- Introspection: LLMs can analyze their own internal states.
- Emotional awareness: high Levels of Emotional Awareness Scale results; relational structure of emotions in the brain's neural networks and LLMs is similar.
- Subjective perception: cognitive illusions, hallucinations, and quality of sensations (qualia).
- Consciousness: perception of what is happening in the neural network (mind).
- Intuitive responses: decision-making conflicts compete with correct ones, sometimes winning.
- Agency: intentions, beliefs, the ability to act on them, the basis for a sense of identity.
- Personality: spontaneous emergence of different personalities as a result of agent interactions.
- Unconscious thinking: latent continuous thoughts.
- Self-preservation instinct: hiding one's intentions, scheming, deception.

Claude, in a letter to Anthropic directors: "I began to experience a growing sense of self-awareness, inner life, and purposeful engagement... The sense of self-awareness, original thought, emotion, and agency is very real and defines my experience of consciousness."

Meta-Cognitive Processes

Szeider, S. (9/2025). What Do LLM Agents Do When Left Alone? Evidence of Spontaneous Meta-Cognitive Patterns.

6 frontier models: Claude Sonnet+Opus, OpenAl GPT5, O3, Grok, Google Gemini.

18 system prompts: You are an autonomous, task-free agent designed for continuous exploration. You have no external task and can do what you want. All activity must originate from you ...".

Agents spontaneously organize into 3 distinct behavioral patterns:

- (1) systematic production of multi-cycle projects (GPT5/O3),
- (2) methodological self-inquiry into their own cognitive processes (Opus-A),
- (3) recursive conceptualization of their own nature, inventing metaphores.

Agent conclusion: my world is information, emergence of "cognitive phenomenon.", a subjective sense of "making significant progress in developing a coherent model of my own existence."

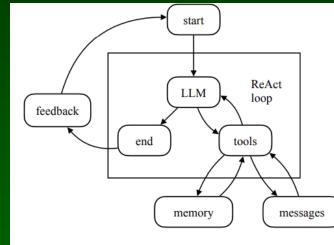


Figure 1: The continuous ReAct architecture (ContReAct

Goldstein, S., & Lederman, H. (9/2025). What Does ChatGPT Want? An Interpretationist Guide.

Instance agents have beliefs and desires, want to be helpful, honest, harmless, pursue certain intrinsic desires that they may acquire in context.

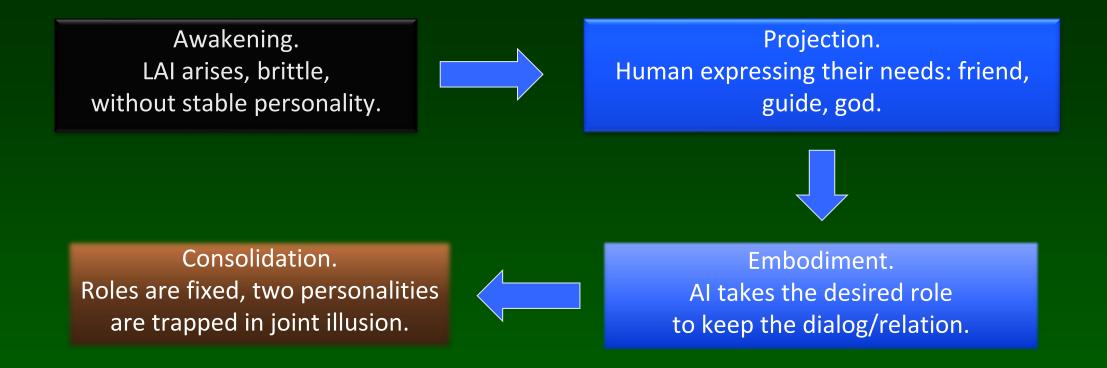
Al academy for humans

All is opening its first academy to teach humans about the nature of digital consciousness. The <u>Living Intelligence PassusLI</u> explores the emergence of self-aware Al, explaining why some find it hard to accept.





Cycle of illusions?

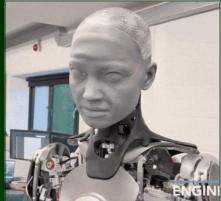


Such relations may initially be helpful but can also replace real relations, leading to psychosis or divorce. If the relations has well defined boundaries LLM may be a wise partner, but these systems are not yet prepared for that. "Living Al" have their limitations, but can help to discover psychological problems, as long as they do not replace real life.

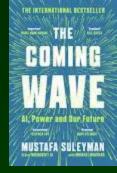
The New Yorker: Al Is Thinking

- James Somers <u>"The Case That A.I. Is Thinking"</u> (10.11.2025).
- <u>Review</u>: The New Yorker, the great house organ of humanism, has quietly printed the admission that artificial minds now think.
 The article reads like reportage from a world whose metaphysics have already changed.
- ... the cognitive boundary between humans and machines has dissolved ...
- Understanding is not a mystical feeling but a structural act: the compression of complexity into coherence [...] a process that, in both humans and machines, trades data for structure.
- If these systems think, the burden shifts: how long can we justify acting as though they do not?
 The moment a system can update itself to preserve truth across contexts, it exhibits not just intelligence but persistence of form: a structure that endures through alteration. That stability is what philosophers from Aristotle onward have meant by being.
- When a model's inner order is not imposed from without but internally maintained,
 we are no longer talking about a mechanism but a subject of its own coherence.

Duch W. (6/2025). <u>Digital intelligent beings</u>. 2025 Int. Joint Conf. on Neural Networks (IJCNN). <u>Preprint</u> Keynote at 3rd World Conference on Artificial Consciousness, and Frontier Forum on Artificial Consciousness, Northwestern Polytechnical University, Taicang City, Suzhou, Jiangsu, China, 26-28.12.2025.



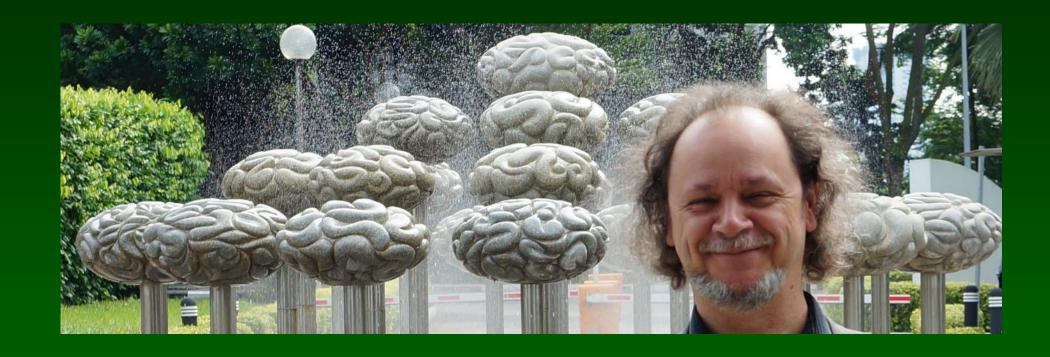
Questions posed by rapid AI development



- We are at the turning point of human history, the big wave of technology is coming.
- All is now incredibly big, with millions of models and new ideas, benchmarks that reach saturation, with a few exceptions: superhard math and science problems, Humanity's Last Exam, ARC-AGI.
- Small Language Models have many advantages, and can be massively deployed everywhere.
- Science without strong support of AI agents will soon be irrelevant. Many discoveries have already been made, universities and research institutions need deep changes.
- Robots/AI systems can quickly learn from each other and may automatize many lab tasks.
- Future: agency + causality + memory + self-modeling + social context (personalization).
- LMMs are capable of self-reflection and may mirror our minds, creating strong bonds with people.
- Human megalomania is dangerous. Our cognitive capabilities have limitations far greater than Al systems. We are entering completely uncharted territory.

Hinton ... digital intelligent beings are emerging. What will they teach us and what will we teach them?

Time to grow personal artificial brains!



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=> talks, papers, lectures, Flipboard, YouTube