

GENERATIVE AI IN RESEARCH: POTENTIALS AND PITFALLS

Unleashing Computational Creativity in Science

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THE GENAI MOMENT: EXECUTE -> GENERATION

- Early on
 - **automation** and
 - **tools optimized efficiency,**
- **Now**
 - **generation of “something” new**



FROM SUPPORT TOOL TO ACTIVE PARTICIPANT IN RESEARCH

- MIT uses LLMs to assist in theorem proving opens new logical pathways that humans might overlook.



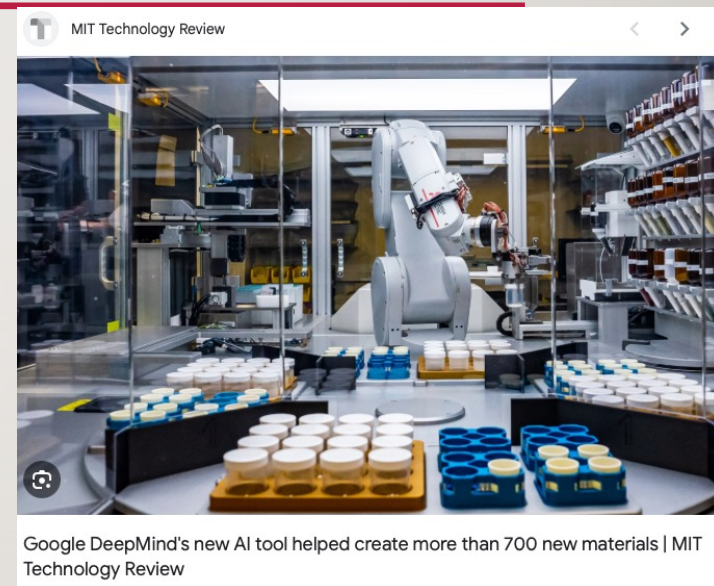
- DeepMind's AlphaFold used AI to predict 200 million protein structures, accelerating decades of biological research

from computation to “creativity”



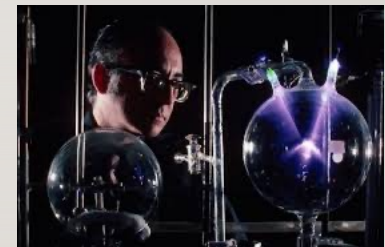
NEW KNOWLEDGE GENERATION: EXAMPLES

- design new materials
 - MIT 700 new materials
- write coherent hypotheses, and
- discover mathematical relationships
- Astrophysics: diffusion models



WHY IT MATTERS FOR RESEARCHERS

- Expands research imagination and productivity
- Automates tedious tasks
- Opens new experimental possibilities
- Democratizes access to advanced modeling



IBM AD -> AI OBJECTIVE



In smarter **research**,
you don't use AI to do what you already do;
you use AI to change what you can do.

IMPLICATIONS FOR US

- **understand many facets** of GENAI use for research
- (may have to) change our **attitude towards how we carry out research**
- requires us to **introduce students to AI-assisted research**
- consider **ethics**
- **avoid potential pitfalls**
- requires us to **learn&teach AI usage** in general (other talk)

FACETS: GENAI FOR CODE AND ALGORITHM GENERATION

- Code completion (e.g., Copilot, Code Llama)
- Auto-generation of test cases and documentation
- Algorithmic exploration
- Debugging suggestions through large code models



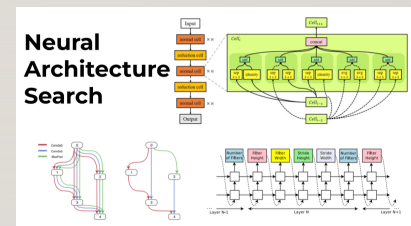
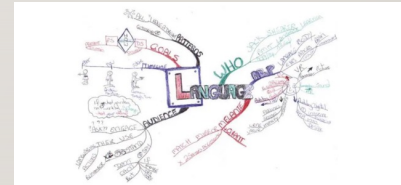
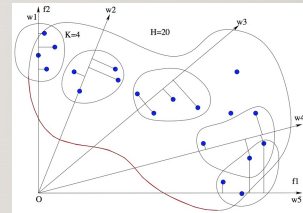
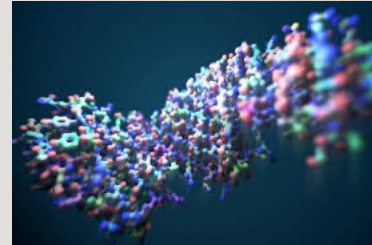
FACETS: GENAI FOR LITERATURE AND KNOWLEDGE DISCOVERY

- **Question answering** over domain-specific papers



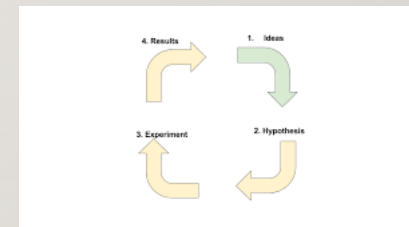
FACETS: CROSS-DISCIPLINARY BREAKTHROUGHS

- Biology: Protein/molecule design
- Physics: Generative surrogates
- Linguistics: Language modeling
- CS: Neural architecture search, code reasoning



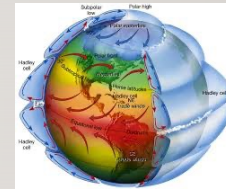
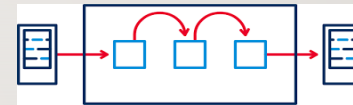
FACETS: GENAI AS A RESEARCH COLLABORATOR

- Brainstorming and ideation
- Drafting hypotheses or abstracts
- Generating alternative experiment designs
- Writing code, documentation, and reviews



RESEARCH COLLABORATOR: EXPANDS HUMAN COGNITION

- AI suggest directions derived from prior **literature** and **cross-domain analogies**
- Climate Science: new model parameterizations for global circulation models — **combining physics-based constraints with data-driven insights**
- Social science: researchers use AI to generate **alternative survey questions** or **summarize** qualitative interview data, allowing **faster iteration cycles** and **richer data interpretation**

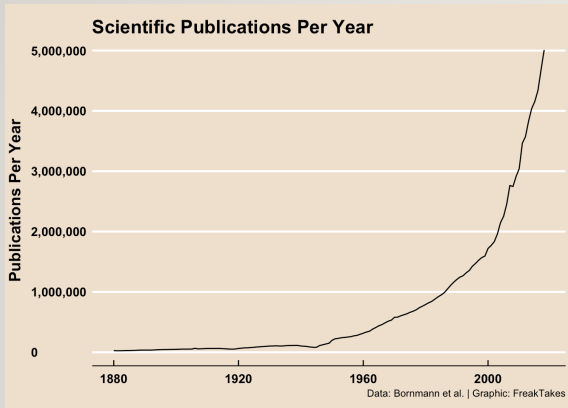


	New edition	Substantive updates	Minor updates	Minor updates	New edition
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FACETS: GENAI FOR LITERATURE AND KNOWLEDGE DISCOVERY

- **Semantic summarization** of individual or large corpora

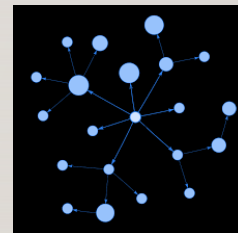


tools: Google NotebookLM,
Elicit, Connected Papers,
Iris.ai, Research Rabbit



- **Concept graph** extraction

tools: Knowledge Graphs and GenAI, Relevance AI,
Notably.ai, IBM Text Mining, ScopusAI



NEW RESEARCH-AI TOOL

(RELEASE END OF NOVEMBER)

Elsevier: **end-to-end AI-powered solution** - spans the full workflow— from idea generation, literature synthesizing, collaborator finding and funding discovery—to accelerate research while maintaining integrity and trust.

Ideation

Generating new research ideas, identifying gaps, and shaping overall objectives

Research planning

Literature review, hypothesis formulation, and outlining protocols or experiments

Analysis & write-up

Analyzing data, Writing up methods, results, and conclusions; drafting formal scientific outputs

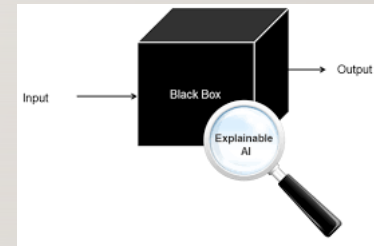
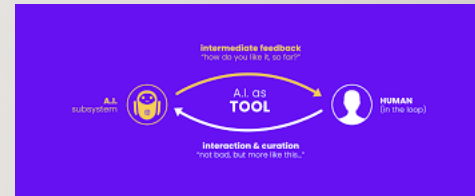
Securing funding

Securing resources, planning budgets, and engaging with funders or management

Declaration: I am involved

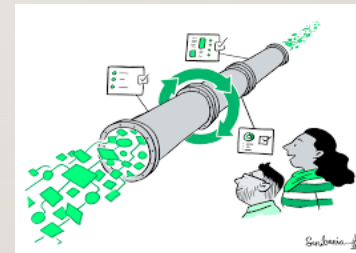
RESPONSIBLE ADOPTION

- Maintain human-in-the-loop
- Promote open benchmarks
- Develop explainable AI
- Institutional GenAI policies



THE ROAD AHEAD

- Generative AI reshapes research
- Autonomous research agents
- Integration into reproducible pipelines
- Shared ethical standards



QUESTIONS?
