Artificial intelligence in science: challenges, opportunities and the future of research

GTIPA Summit
Innovation and Competitiveness

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Artificial Intelligence in Science

CHALLENGES, OPPORTUNITIES AND THE FUTURE OF RESEARCH

OECD

Today's presentation

The context : why AI in science matters

AI in science today and tomorrow

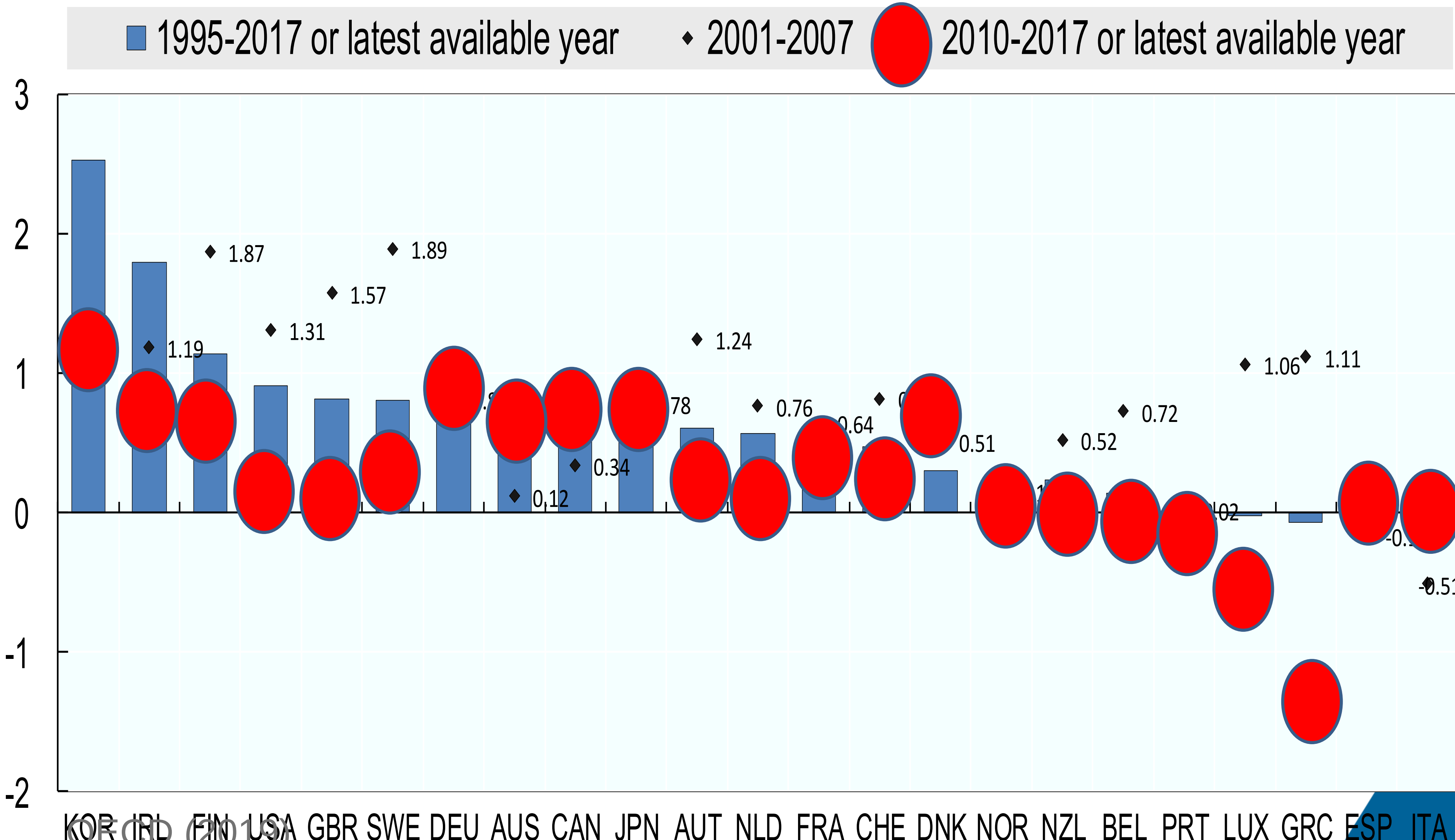
Impacts of AI in science so far

Public policy and universities

The context

1. WHY BETTER SCIENCE MATTERS

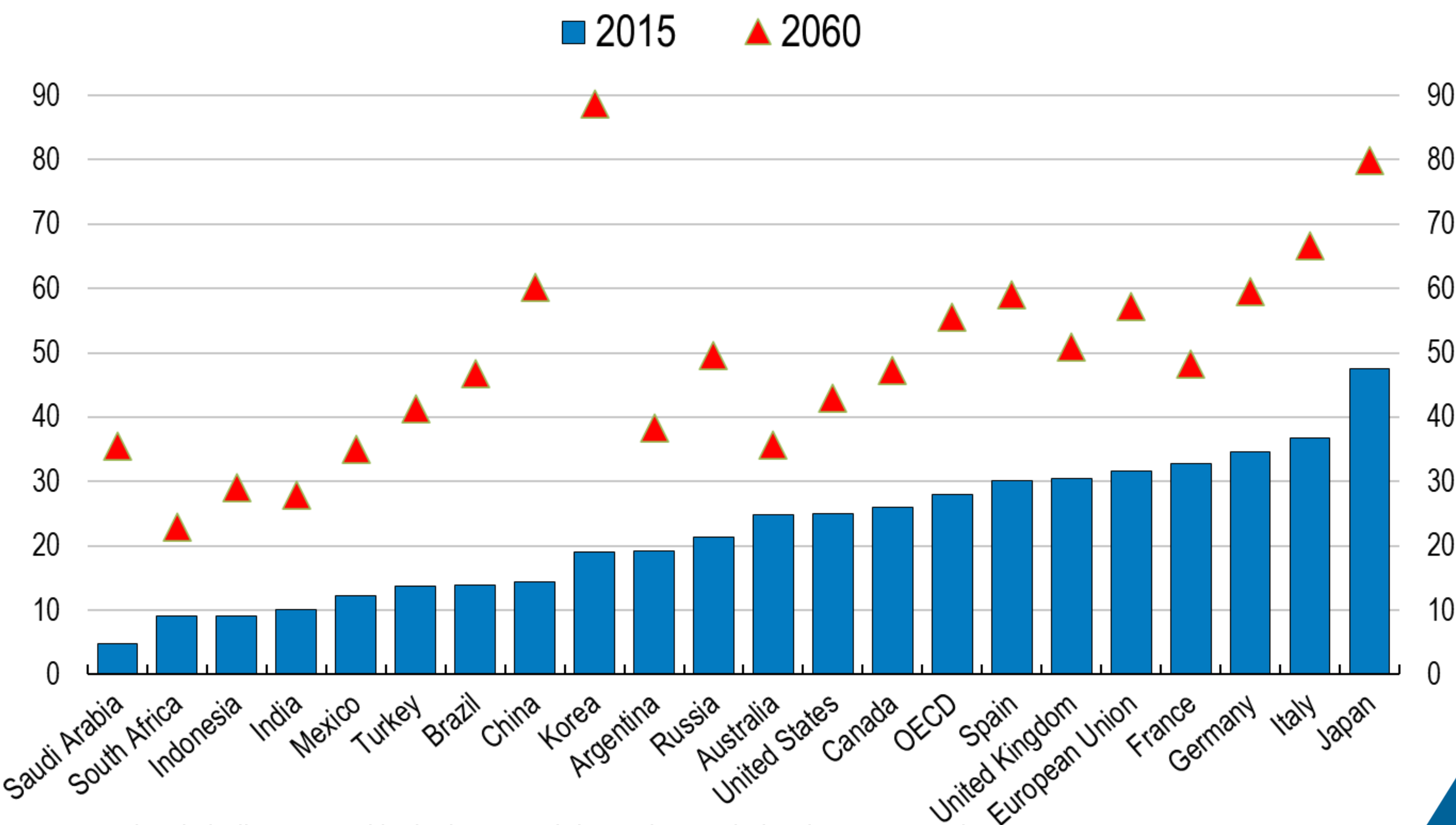
Slower growth of total factor productivity



OECD (2019).

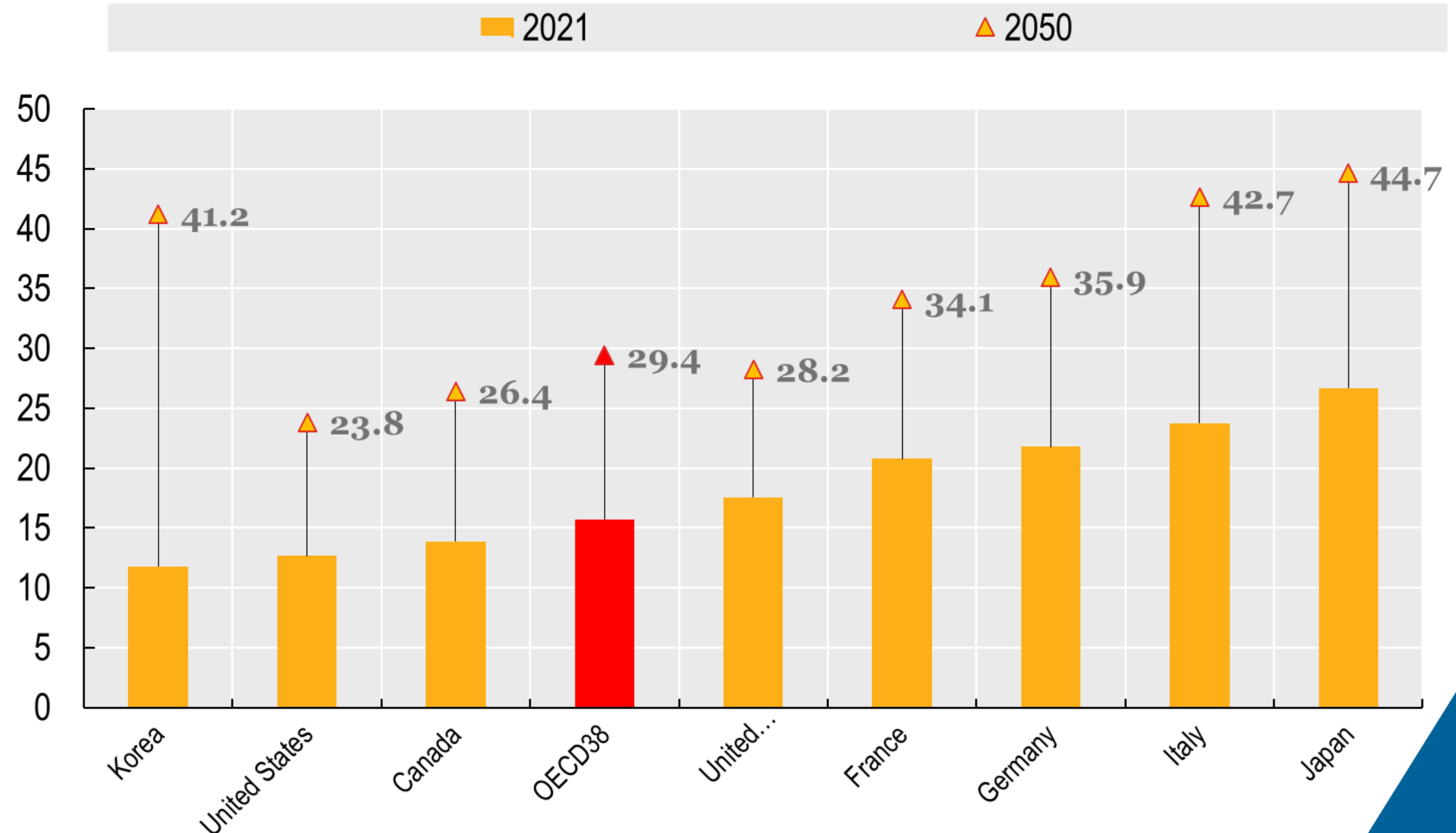
Old-age dependency ratios are projected to at least double in most G20 countries by 2060

Number of people older than 65 years per 100 of working-age (20-64)



Source: Fiscal challenges and inclusive growth in ageing societies (OECD, 2019)

People with dementia per 1000 population, 2021 and 2050



Source: Health at a Glance (OECD, 2021)

Breakthroughs in climate-relevant fields, such as materials science

Ultra-light materials – possible uses in improving fuel efficiency in aerospace

Willow glass – strong flexible ultra-thin glass, for low-cost solar cells

But are we facing a slowdown in research productivity ?

Is science getting harder ?

And recent attention to the productivity of research spurred by

the NATIONAL BUREAU of ECONOMIC RESEARCH

Are Ideas Getting Harder to Find?

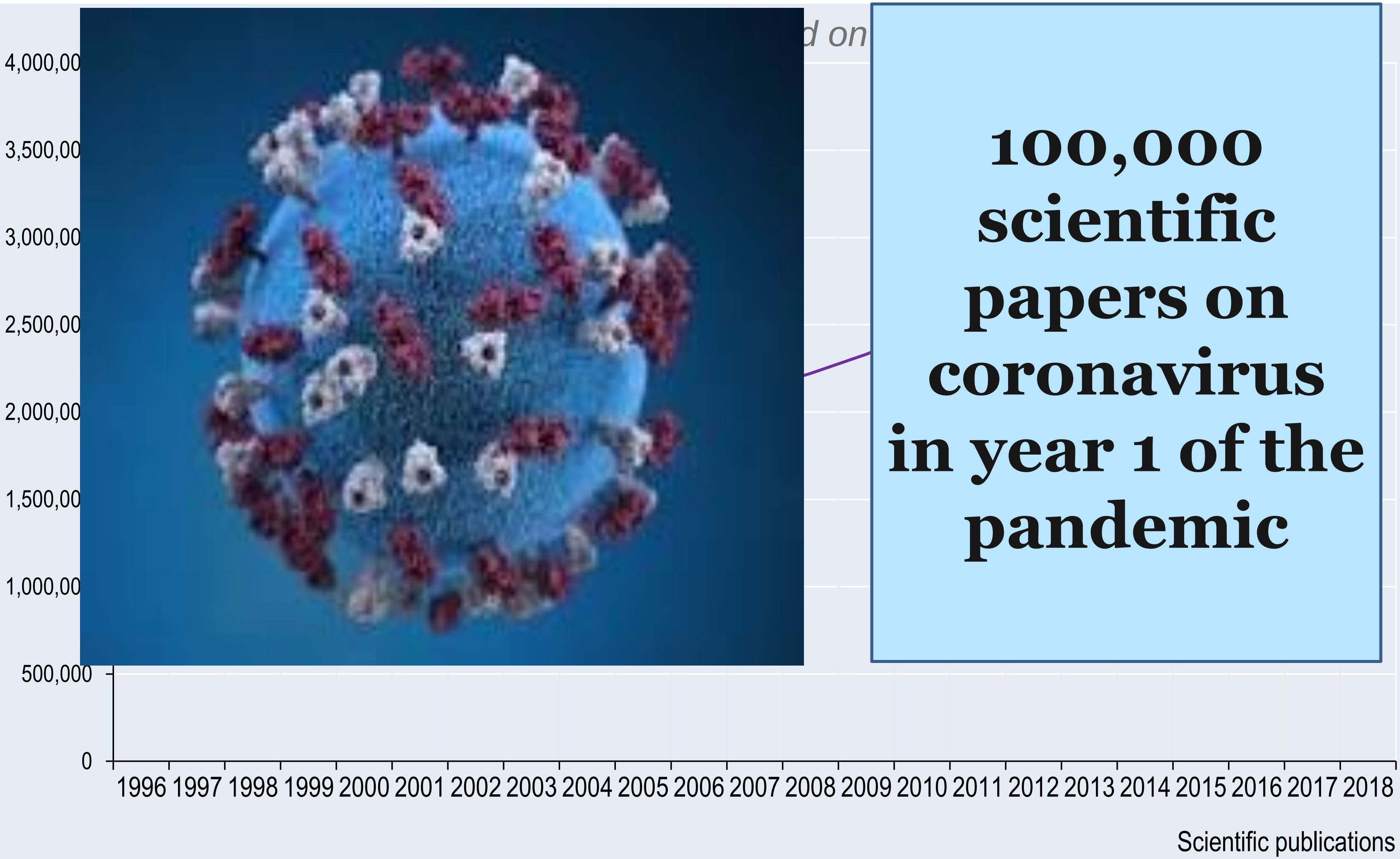
Nicholas Bloom, Charles I. Jones, John Van Reenen, Michael Webb

NBER Working Paper No. 23782
Issued in September 2017
NBER Program(s): Economic Fluctuations and Growth, Productivity, Innovation, and Entrepreneurship

In many growth models, economic growth arises from people creating ideas, and the long-run growth rate is the product of two terms: the effective number of researchers and their research productivity. We present a wide range of evidence from various industries, products, and firms showing that research effort is rising substantially while research productivity is declining sharply. A good example is Moore's Law. The number of researchers required today to achieve the famous doubling every two years of the density of computer chips is more than 18 times larger than the number required in the early 1970s. Across a broad range of case studies at various levels of (dis)aggregation, we find that ideas — and in particular the exponential growth they imply — are getting harder and harder to find. Exponential growth results from the large increases in research effort that offset its declining productivity.

Information overload

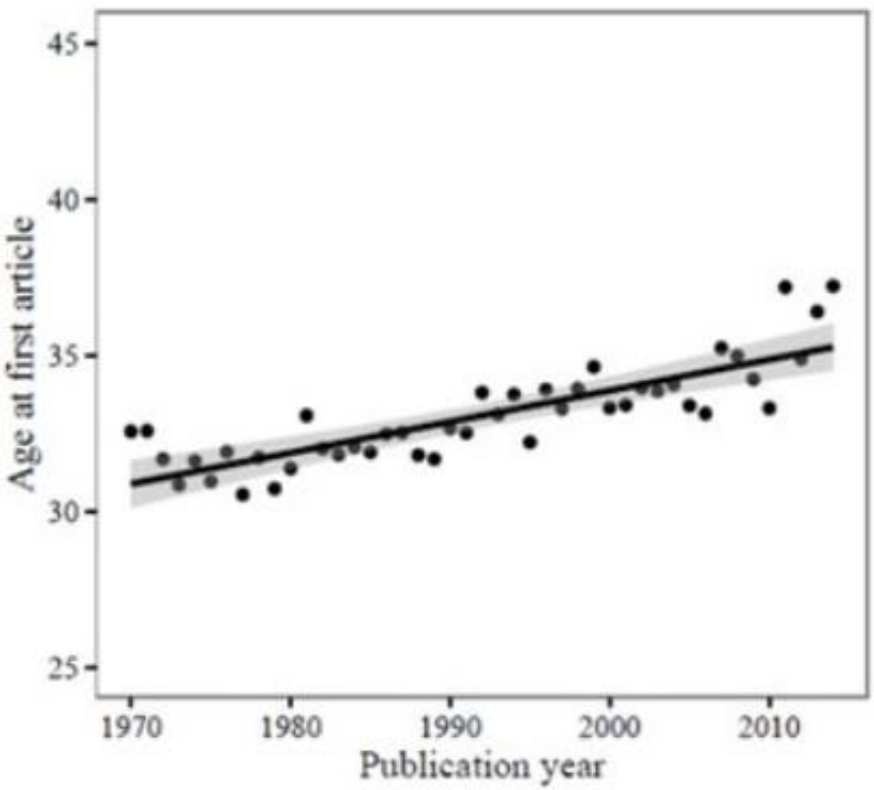
(annual number of scientific publications, 1996-2018)



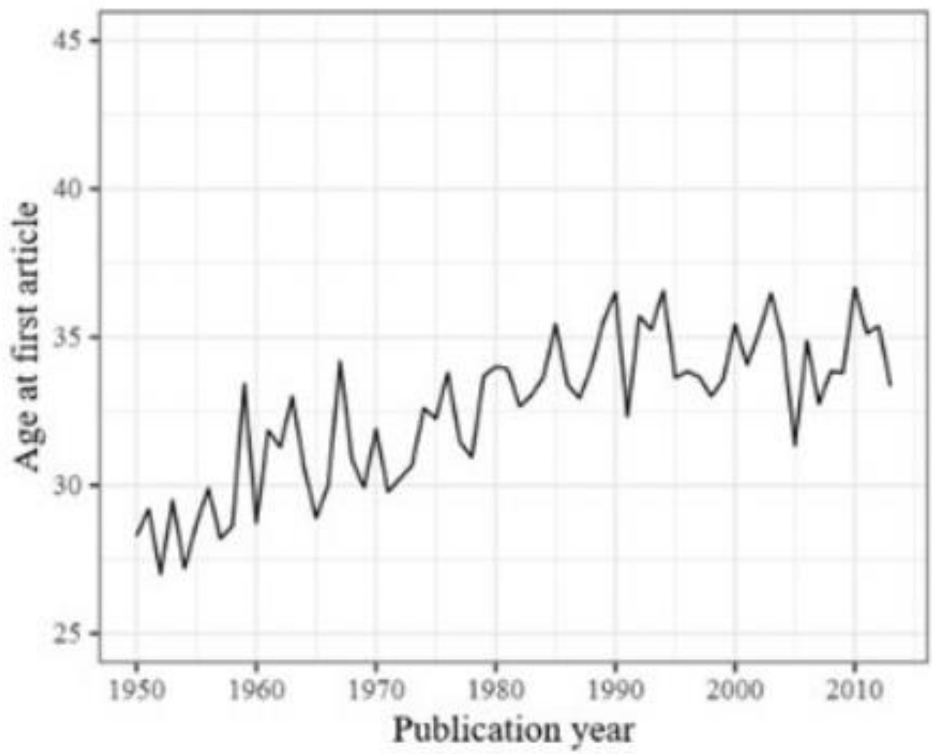
100,000 scientific papers on coronavirus in year 1 of the pandemic

Creating a knowledge burden ?

Age at first solo economics article



Age at first solo (top) mathematics article



Schweitzer and Brendel (2020) Brendel and Schweitzer (2019)

Discovery getting harder ?

$$F = m \times a$$

1686

$$\ln\frac{K_2}{K_1} = \frac{-\Delta H^{\emptyset}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

1884

$$\left(1 - e^{-2\Delta}\right) r^{D-3} = \frac{2\kappa}{D-2}\int_0^r \rho(r') r'^{D-2}\, dr' = \frac{2\cdot 8\pi(D-3)G}{(D-2)}\frac{M}{\Omega_{D-2}} \Rightarrow$$

$$\Rightarrow \frac{1}{3}\frac{4\left[anti\log\frac{\int_0^\infty \frac{\cos \pi x w'}{\cosh \pi x} e^{-\pi x^2 w'} dx}{e^{-\frac{\pi t^2}{4}w'}\varphi_{w'}(itw')}\right]\cdot\frac{\sqrt{142}}{t^2 w'}}{\log\left[\sqrt{\left(\frac{10+11\sqrt{2}}{4}\right)} + \sqrt{\left(\frac{10+7\sqrt{2}}{4}\right)}\right]}. \quad (2.93c)$$

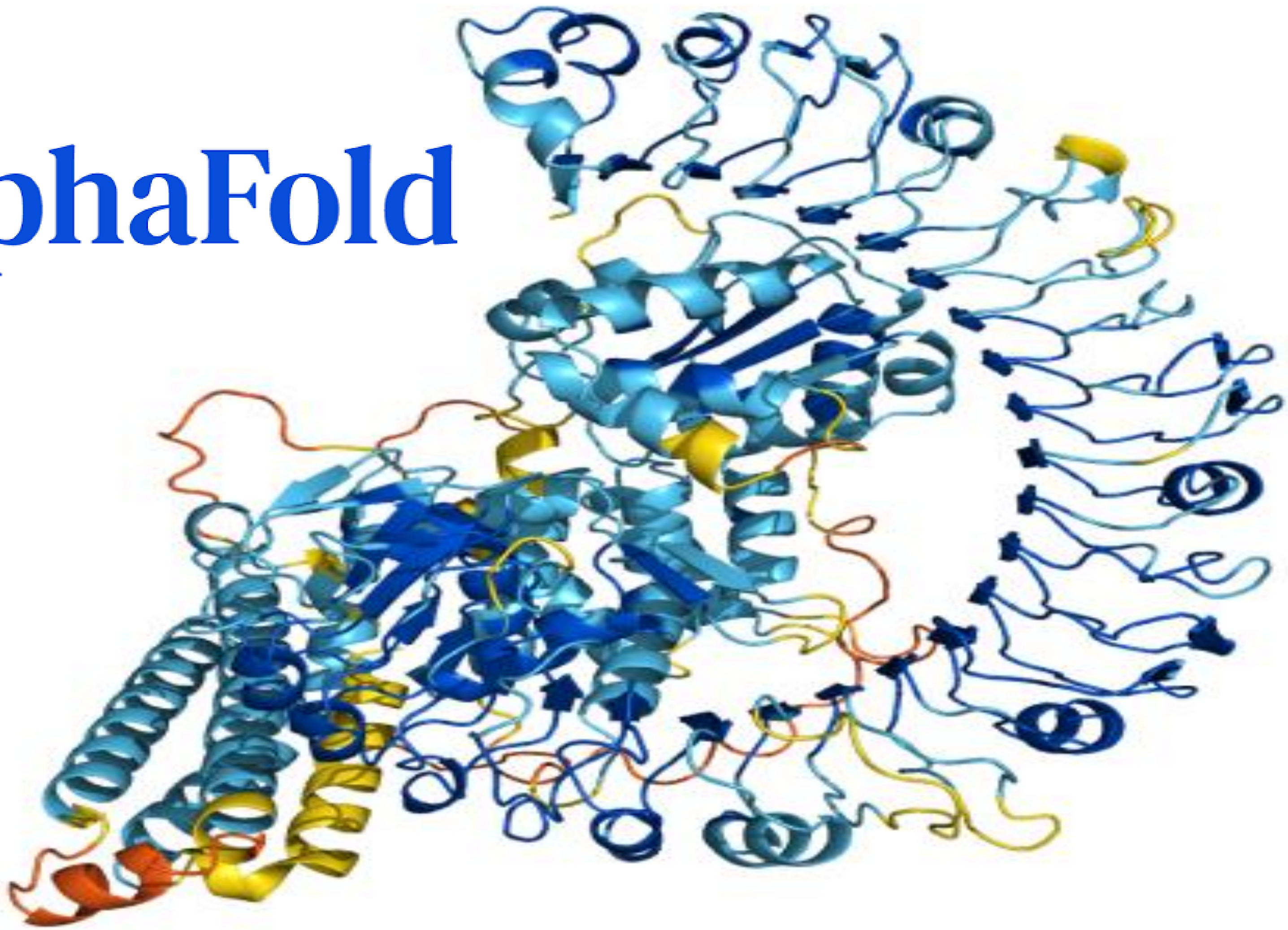
1973

Thanks to Prof. Hugh Cartwright, Oxford University

AI : Coming to scientific knowledge in new ways

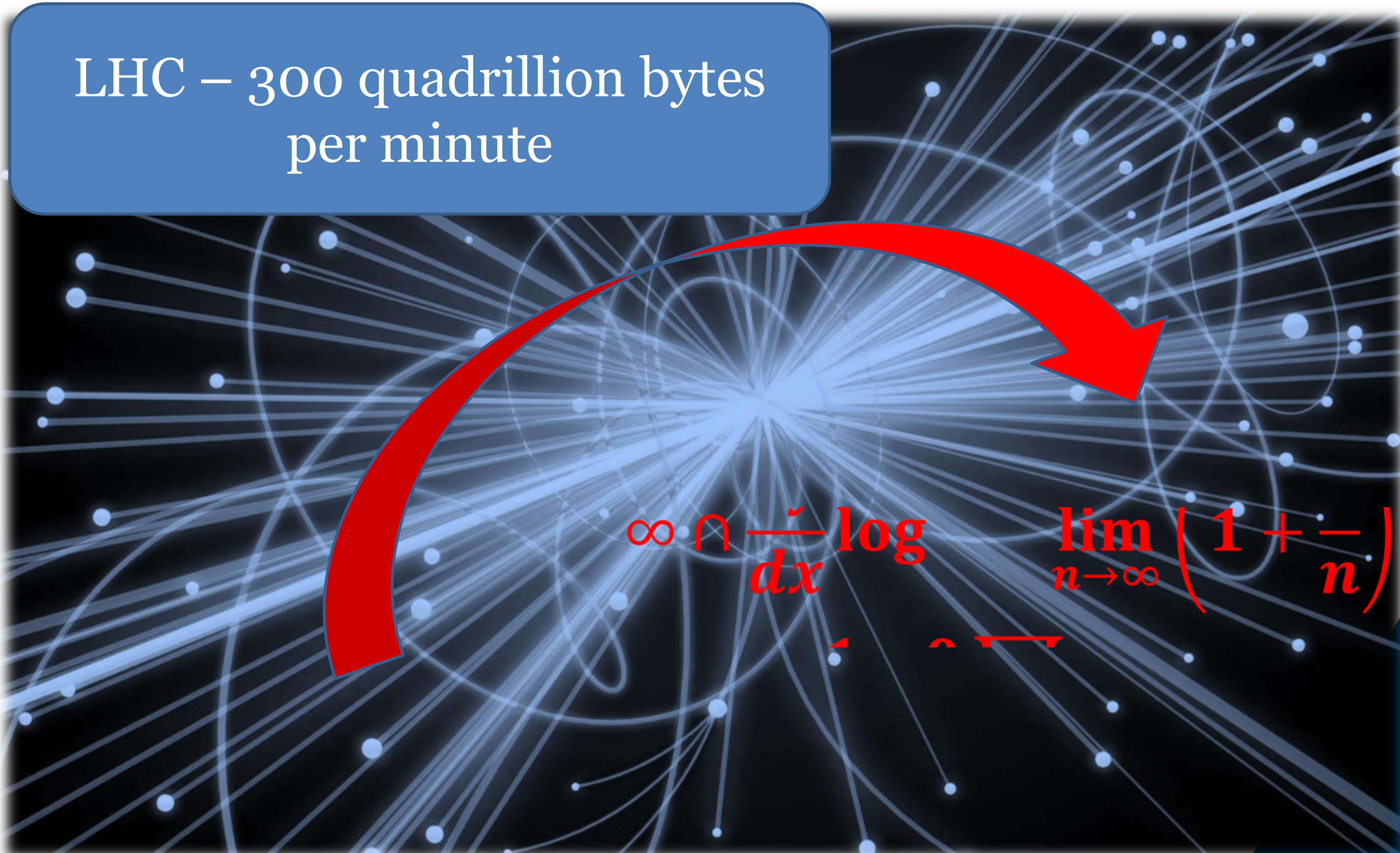
Prediction

AlphaFold

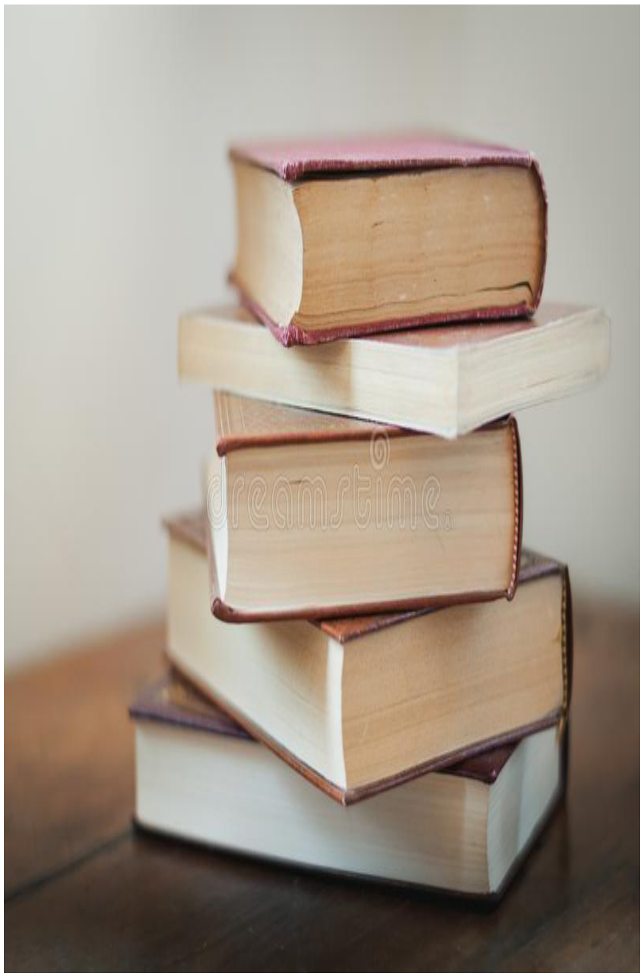


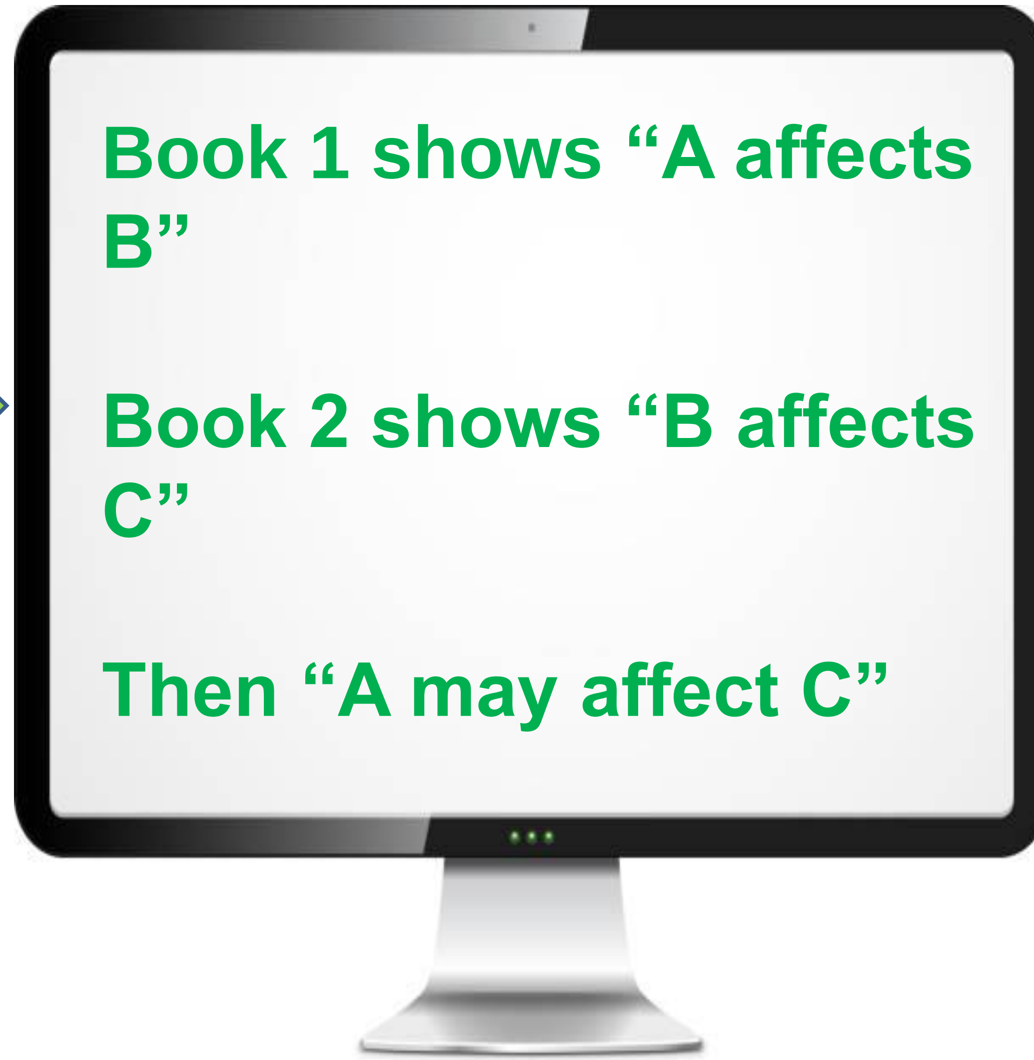
Generating hypotheses from vast datasets

LHC – 300 quadrillion bytes per minute



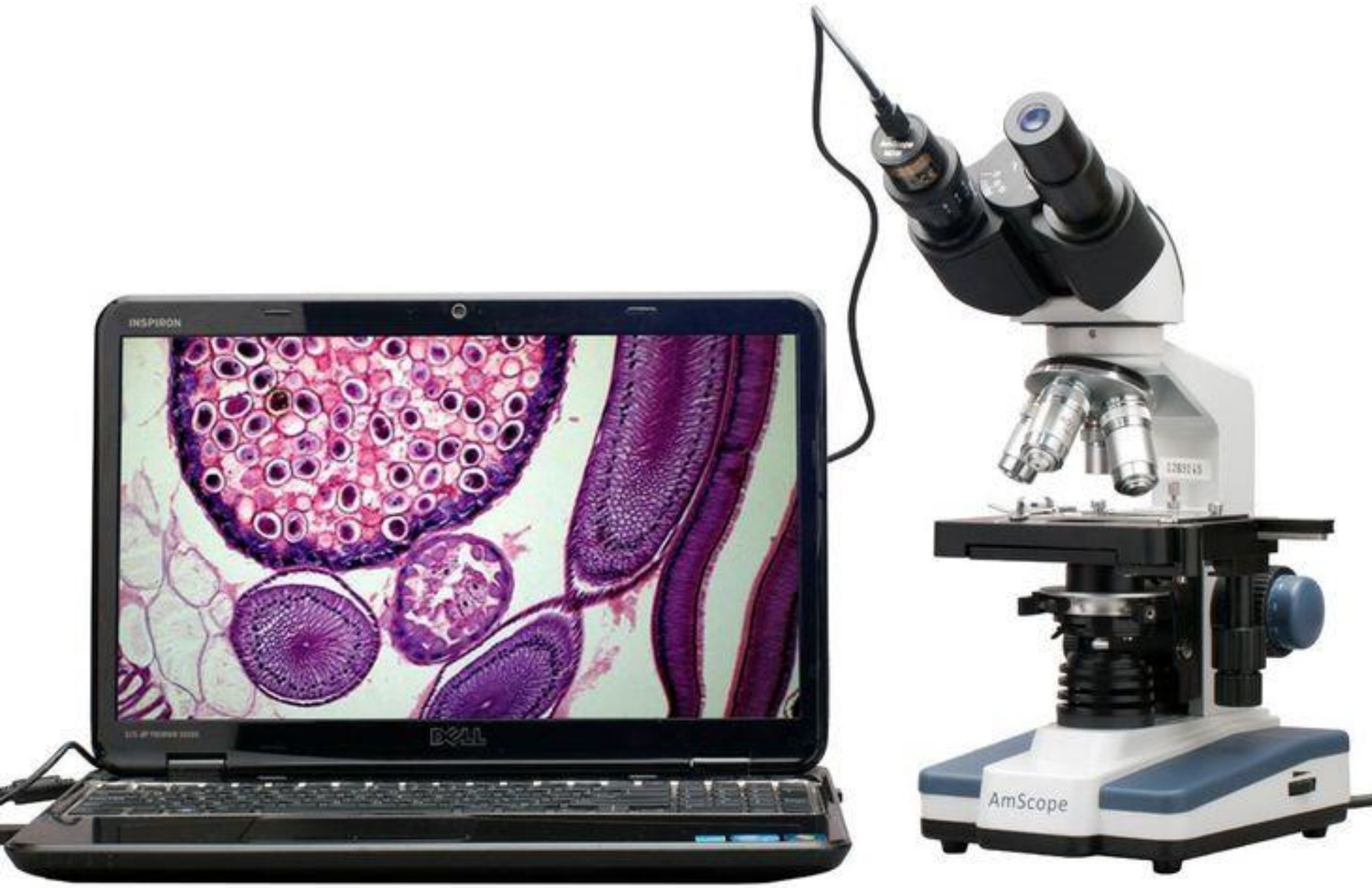
Finding undiscovered public knowledge (knowledge we don’t know we have)

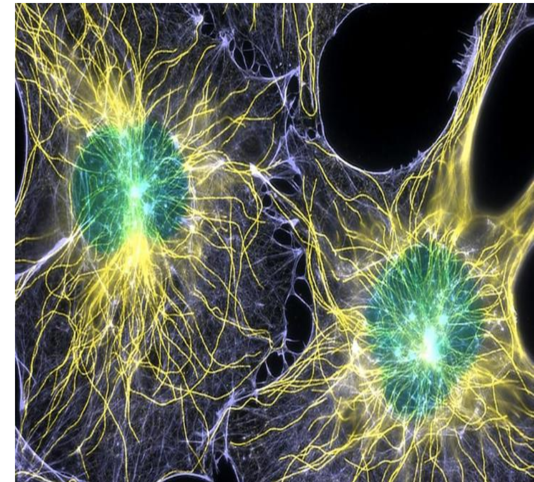




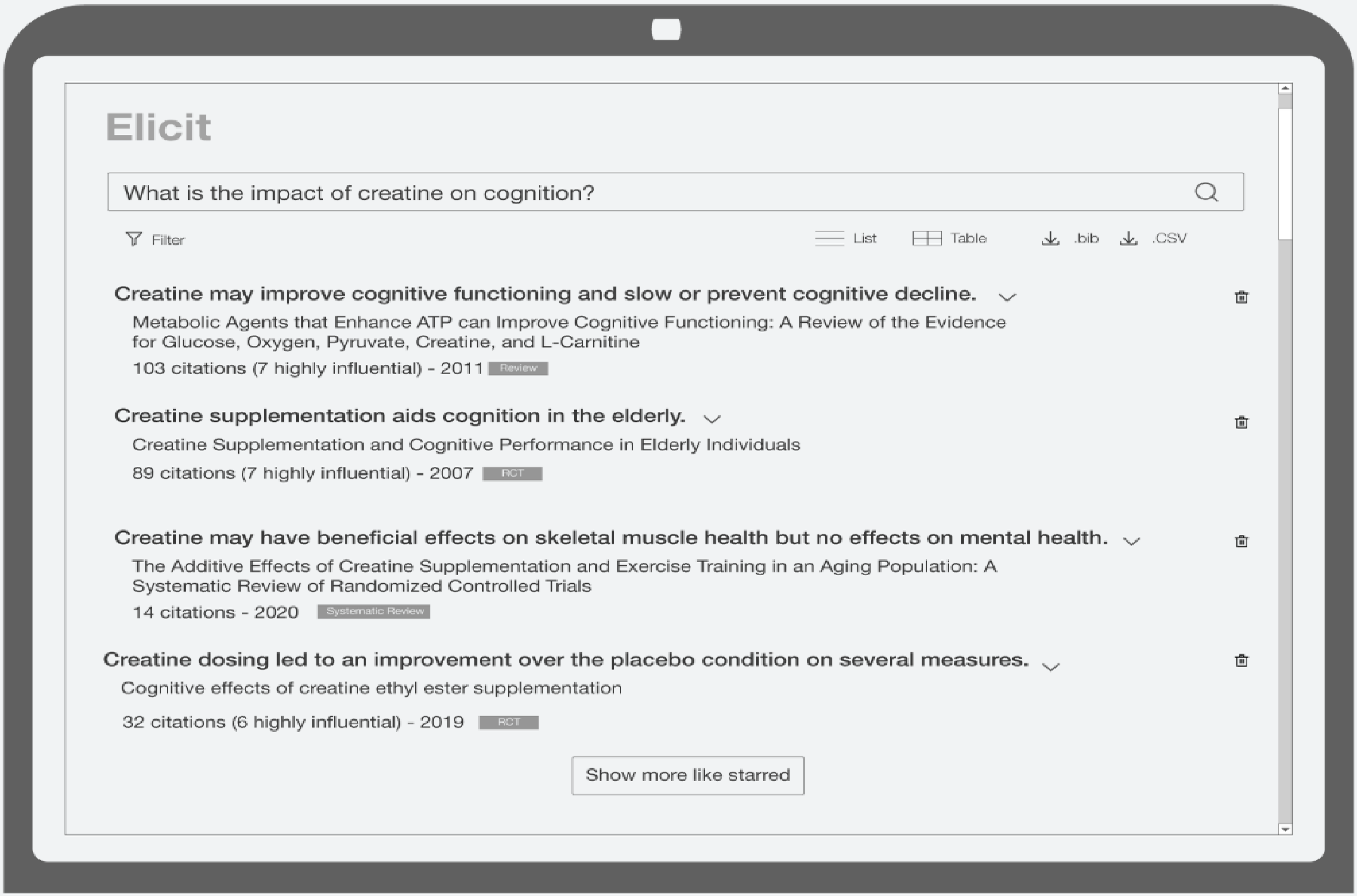
Novel simulation

Revolutionising microscopy





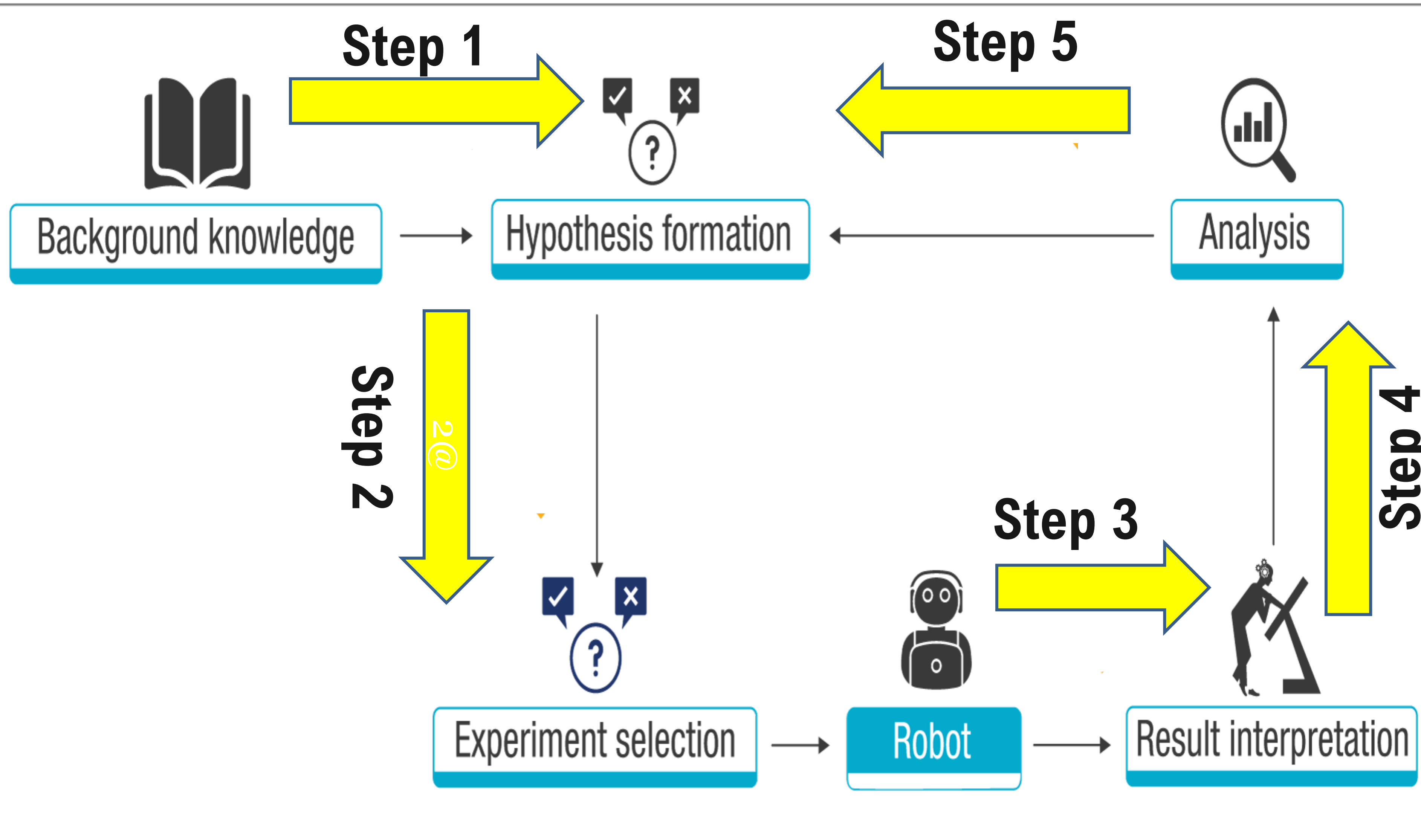
Elicit – (Ought.com) - AI Research assistant – using GPT3



Many other possible AI applications in science

Planning experiments

Robot scientists
Closed-loop cycles of experimentation



Professor Ross King in front of Adam, the robot scientist

Triclosan – works against wild-type and drug resistant Plasmodium falciparum, and Plasmodium vivax.

2008-2015 Eve – Drug Design for Tropical Diseases

Williams *et al.* (2015) *Royal Society Interface*, DOI 10.1098/rsif.2014.1289

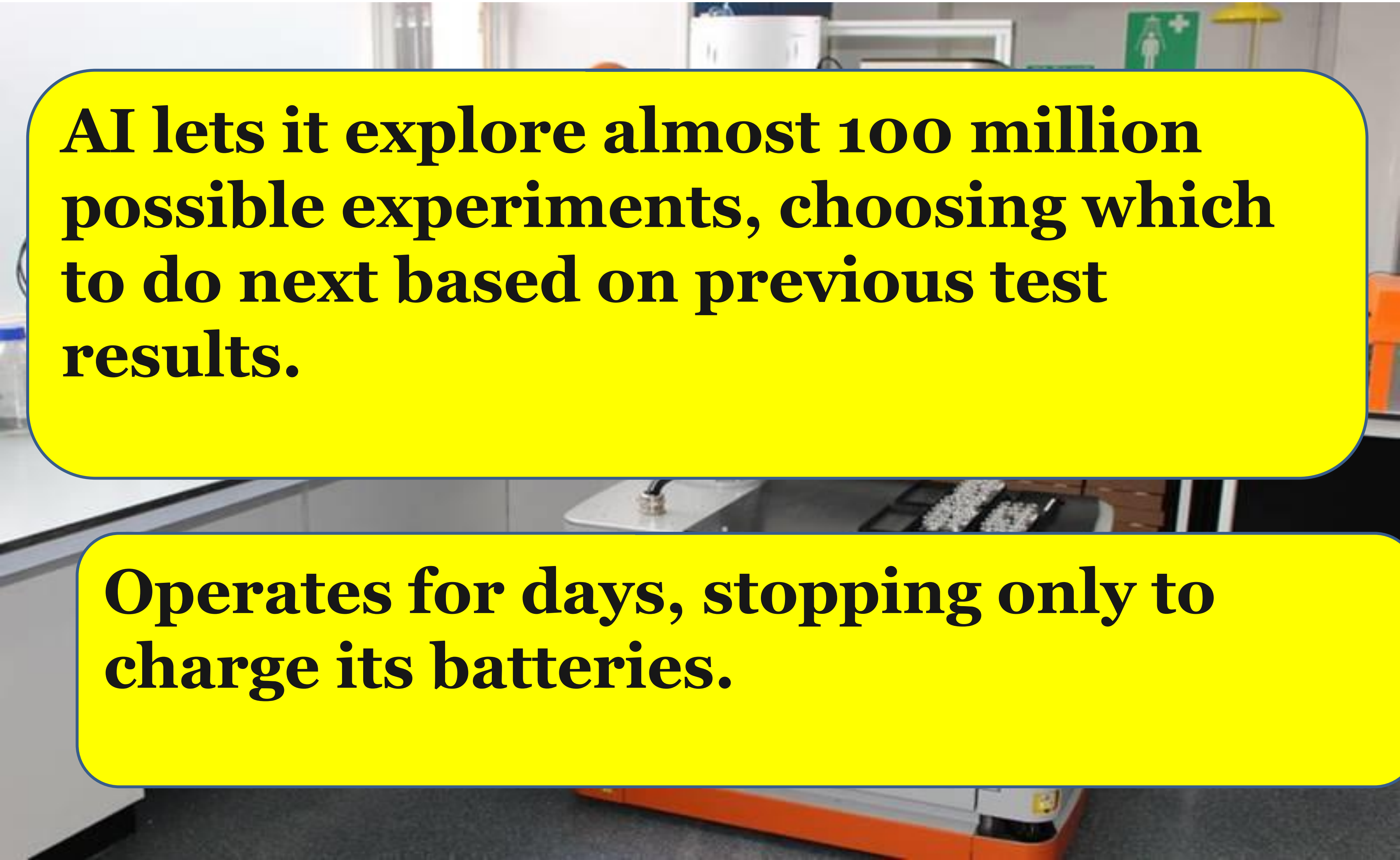
Effects on research productivity ?

Robot scientist
Lowers various types cost

Robot chemist at the University of Liverpool

AI lets it explore almost 100 million possible experiments, choosing which to do next based on previous test results.

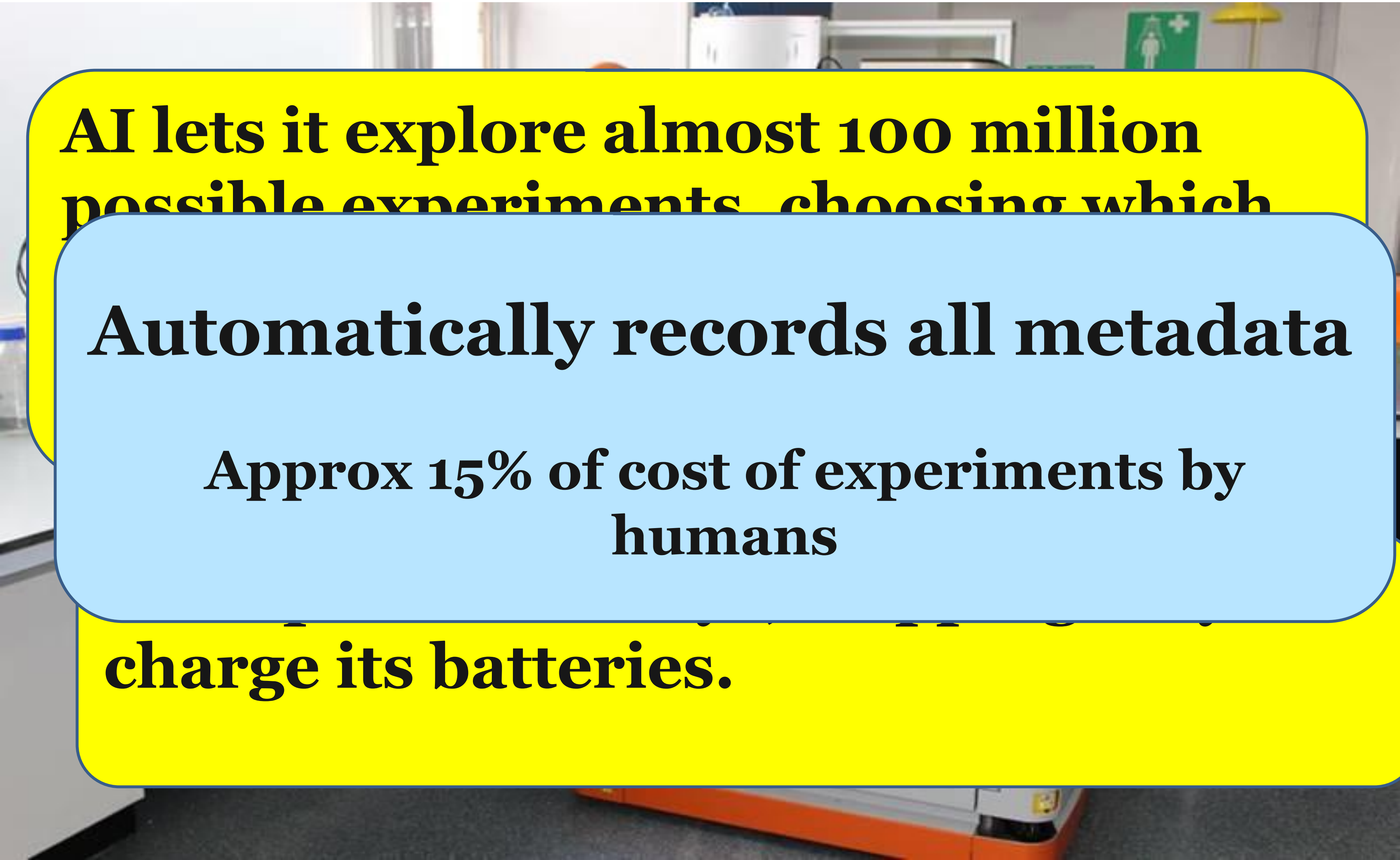
Robot chemist at the University of Liverpool



AI lets it explore almost 100 million possible experiments, choosing which to do next based on previous test results.

Operates for days, stopping only to charge its batteries.

Robot chemist at the University of Liverpool



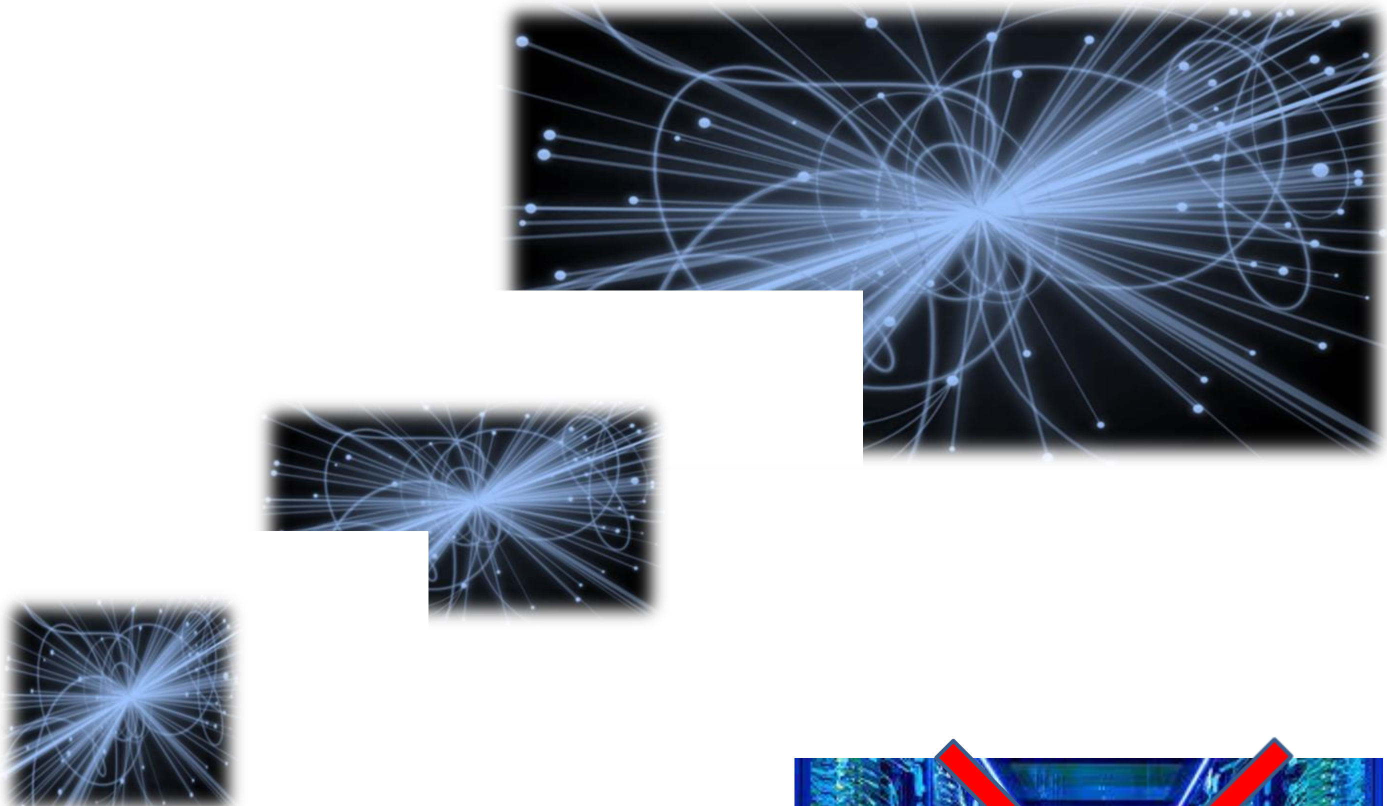
AI lets it explore almost 100 million possible experiments, choosing which

Automatically records all metadata

Approx 15% of cost of experiments by humans

charge its batteries.

Intelligent data sampling saves compute $$$



Intelligent research assistants : to save time and money

8 months to +/- weeks

"Our results show that ChatGPT substantially raises average productivity: time taken decreases by 0.8 SDs and output quality rises by 0.4 SDs."

https://economics.mit.edu/sites/default/files/inline-files/Noy_Zhang_1.pdf

- **USD 1.5 billion in 2020 in the US**

(Aczel, Szaszi and Holcombe, 2021)

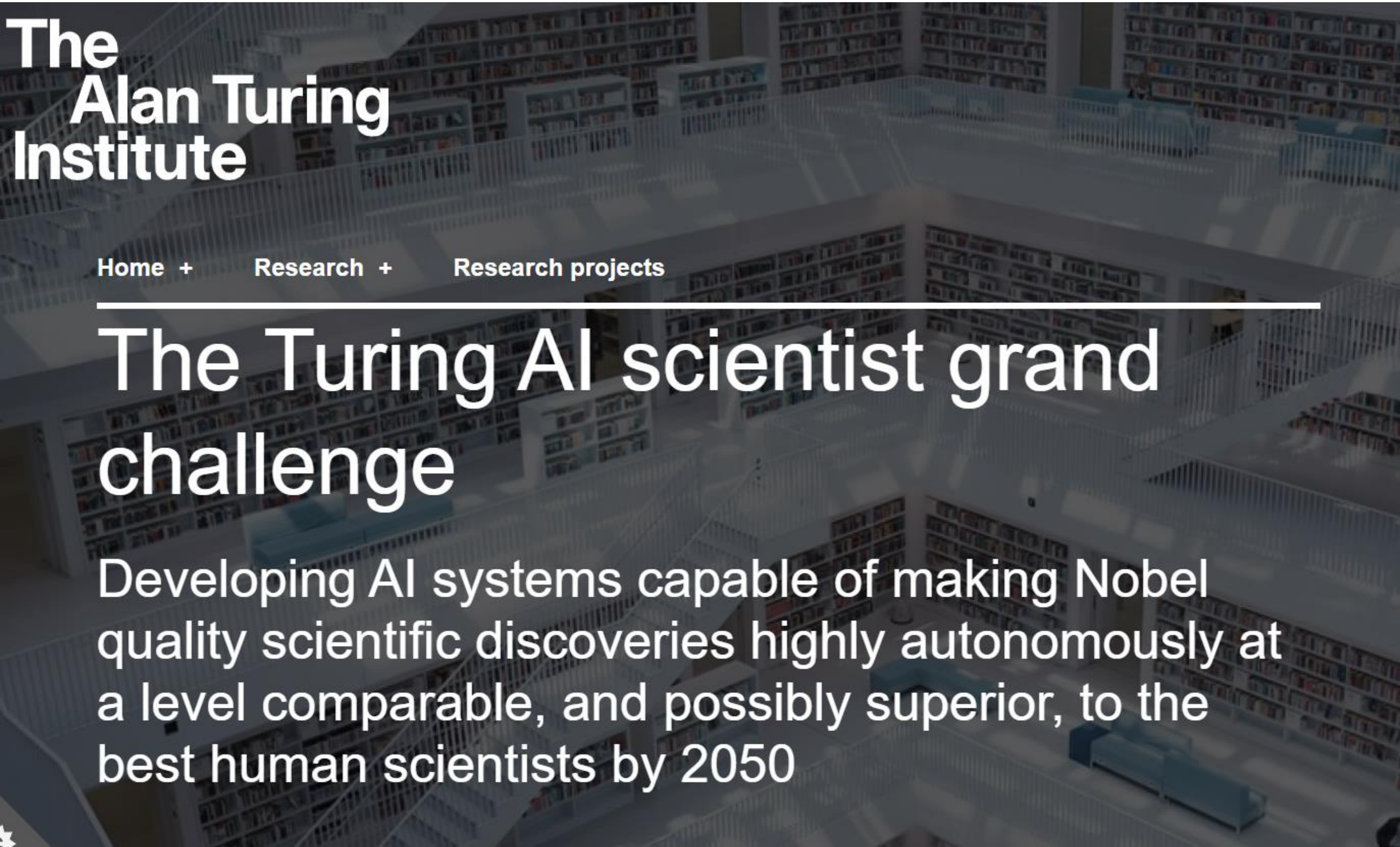
Can public policy help ?

Ambitious multi-disciplinary programmes

Multi-disciplinarity

AI-ML

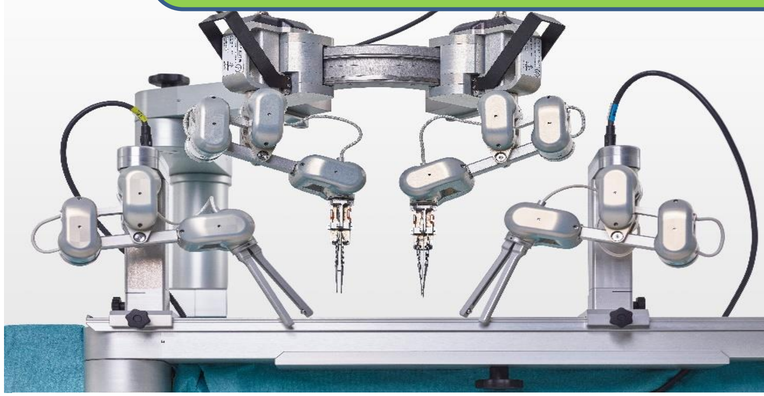
Ambitious multidisciplinary programmes

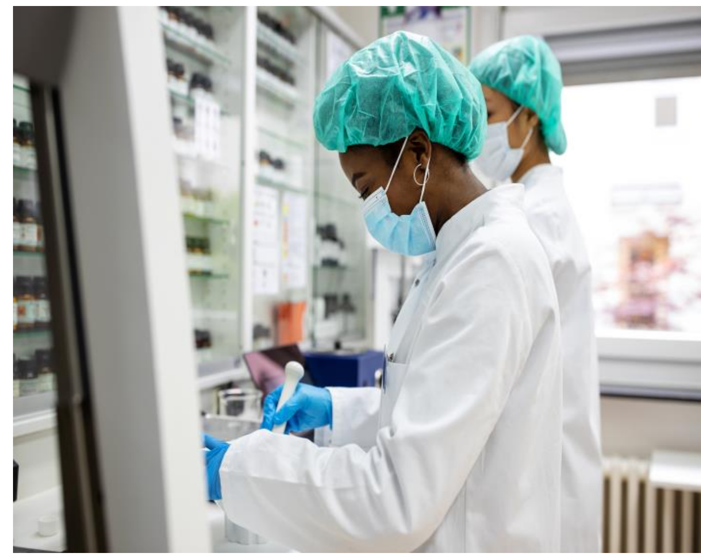


Less than 6% of all LBD publications can be mapped to at least one SDG

Bring industry, roboticists and domain specialists together

Strengthen data governance





Computational resources

- **National labs, industry and academia could work together to nurture AI ecosystems for tertiary education**

Computational resources

- **Na an nu ter**

Explore pooling resources internationally

Curricula

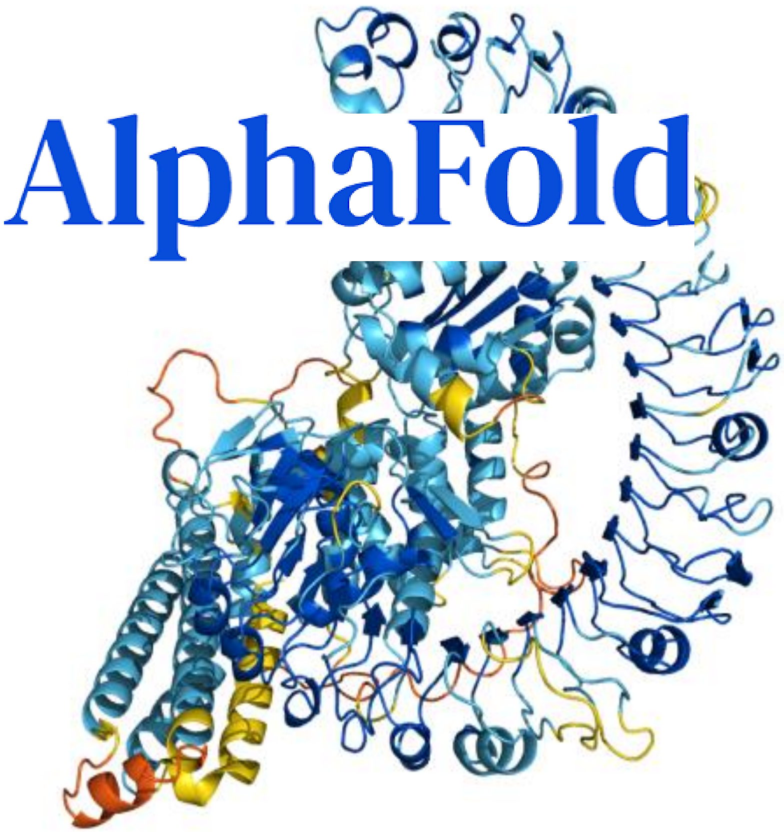
- ***Standard bio-science education doesn't address how to search for new hypotheses.***

- ***New PhD programmes based on knowledge synthesis – aided by AI***

- ***Promote research software engineers and engineering***

Public R&D can advance the field in a variety of ways

Invest in developing new tools for AI in science



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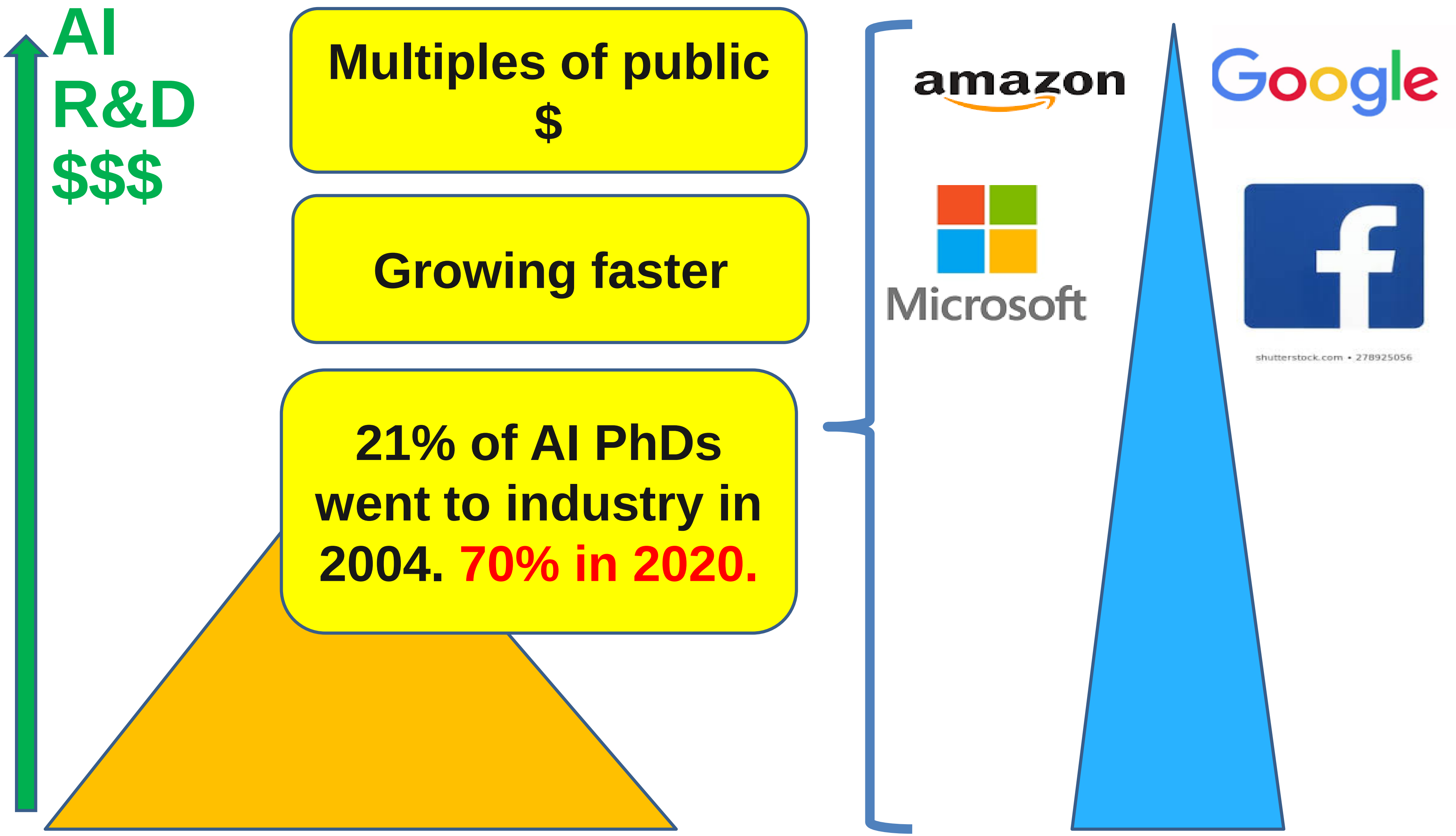
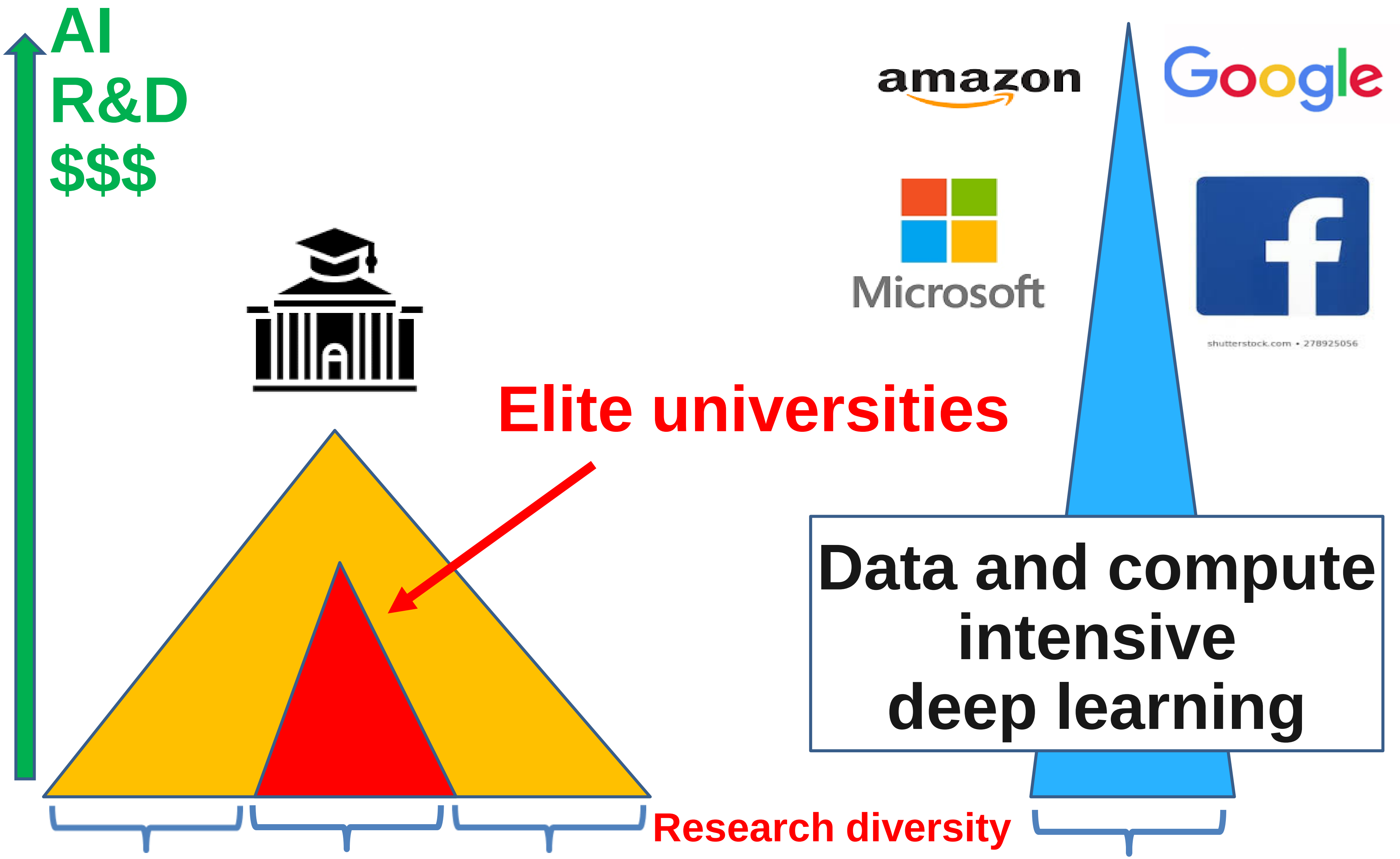
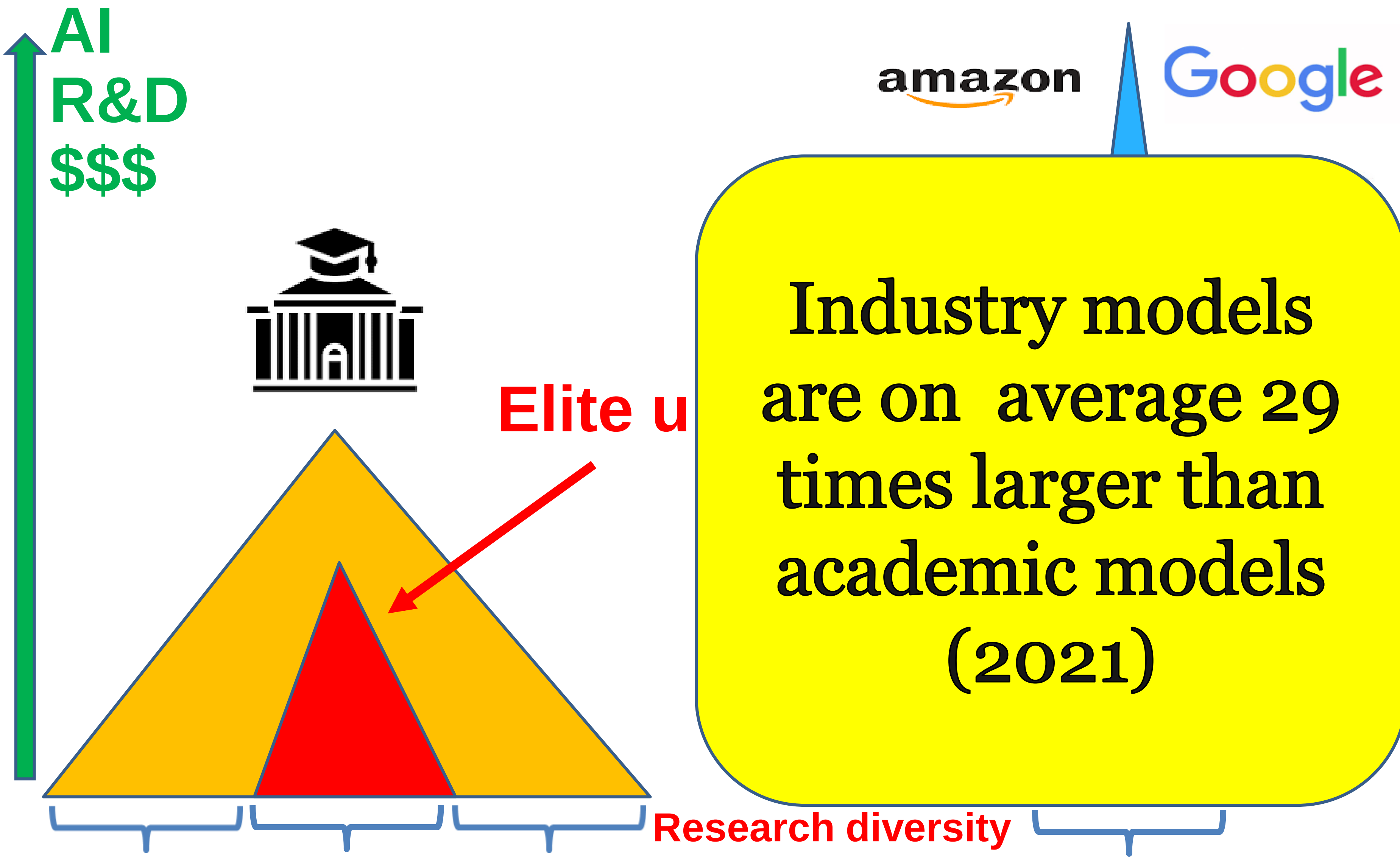
A narrowing of AI research



A narrowing of AI research



A narrowing of AI research



Foster more blue sky thinking

More funding streams and/or publication processes to reward novel methods

Funders could help develop specialised tools to enhance collaborative human AI teams

Research governance

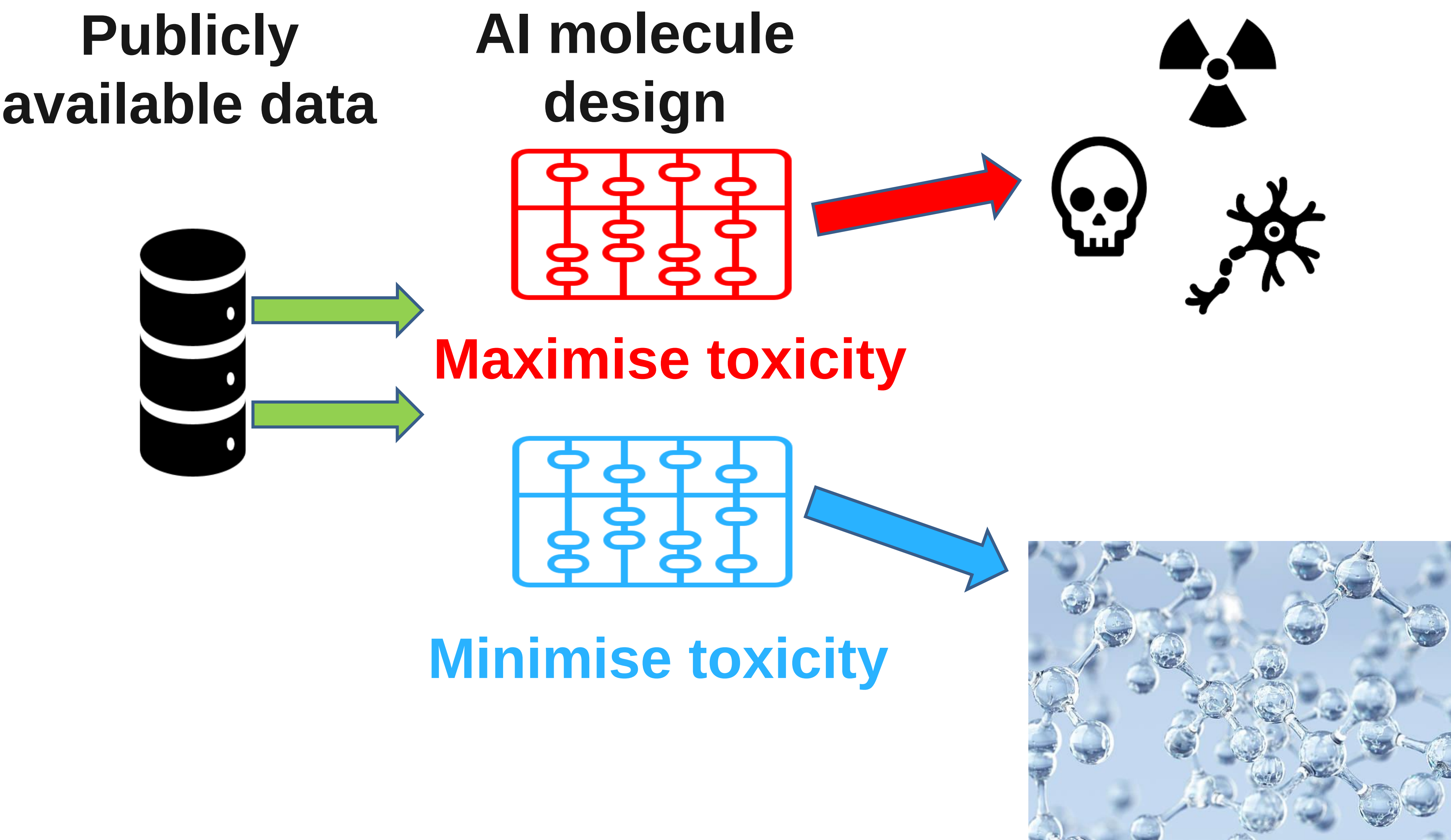
nature

NEWS FEATURE | 06 February 2023 | Correction 08 February 2023

What ChatGPT and generative AI mean for science

Researchers are excited but apprehensive about the latest advances in artificial intelligence.

Dangers of dual use AI in drug design



Dangers of dual use AI in drug design

P

avai

<u>What to do?</u>

- *High-level recognition of this danger is needed*
- *All parts of the science system have a role in responding*
- *Could draw on existing frameworks for responsible science – but technology-specific measures are needed too*

Two parting thoughts

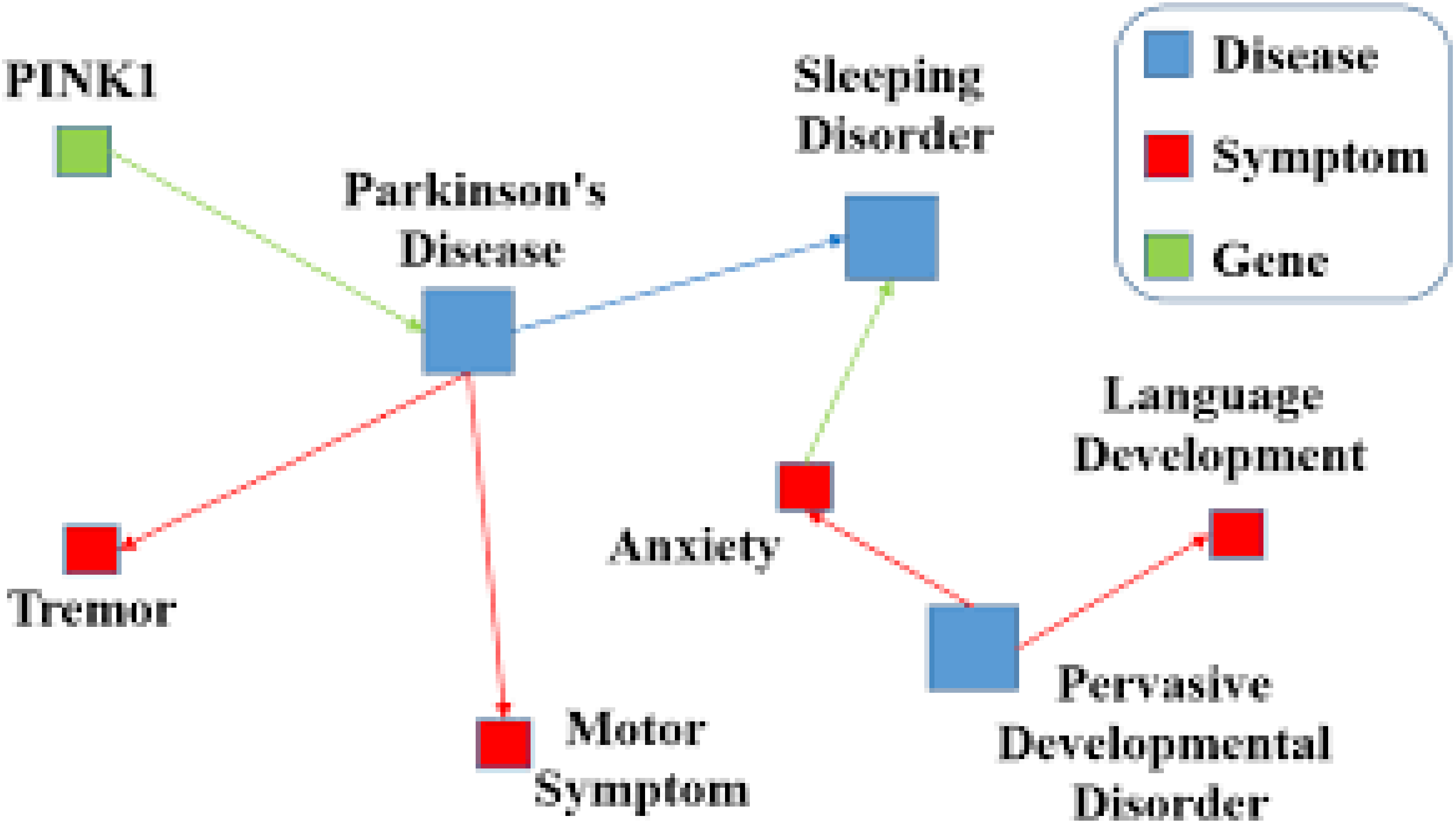
A fast-moving field – much will be new in a year from now.

AI in science may be the most important of all uses of AI.

Thank you

alistair.nolan@oecd.org

Support an extensive programme to build knowledge essential to AI in science

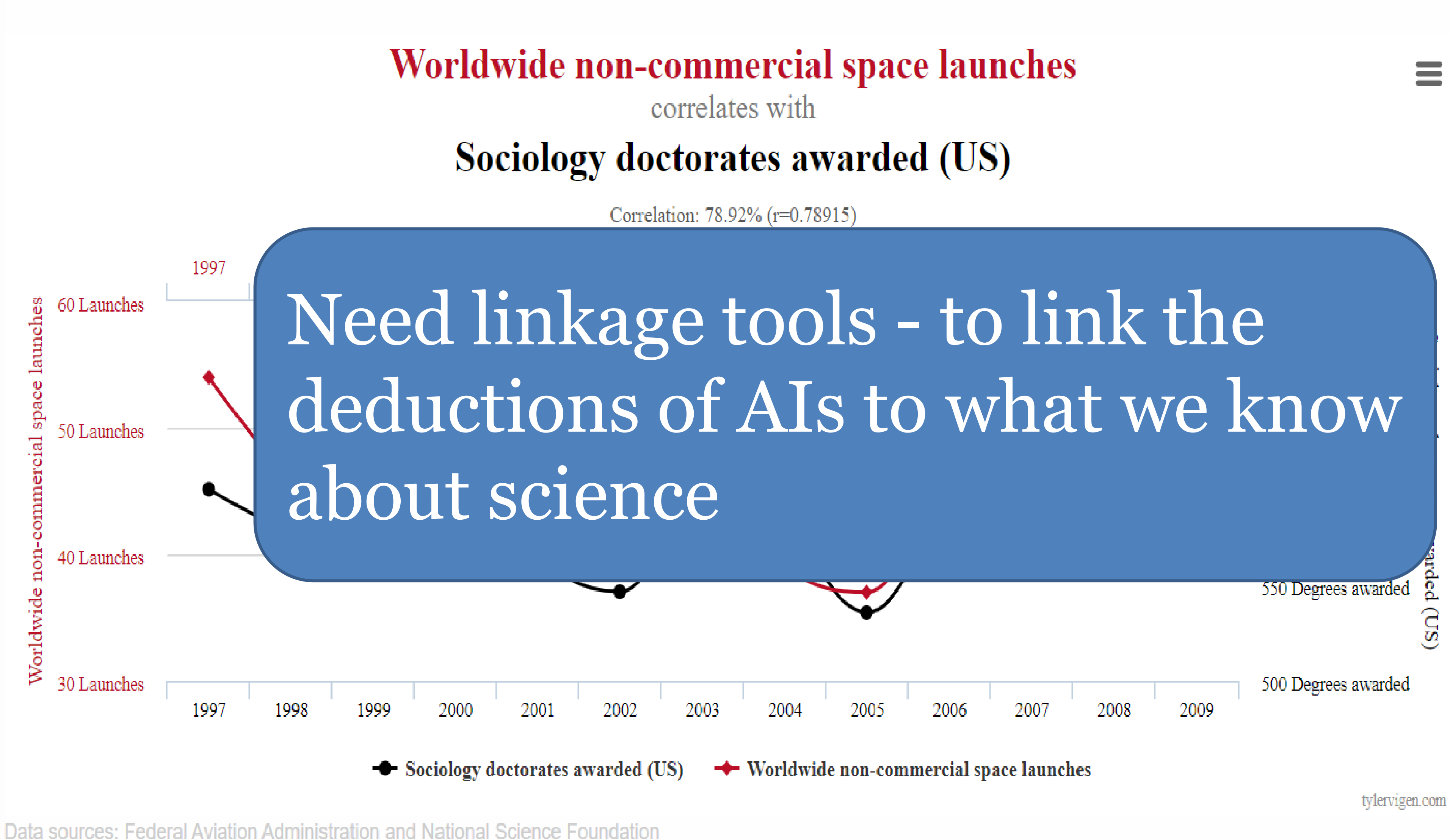


INTERNATIONAL MONETARY FUND

Basic scientific research diffuses to more sectors, in more countries and for a longer time than commercially oriented applied research

2021
OCT

AI in science needs new tools



Need linkage tools - to link the deductions of AIs to what we know about science

What do ChatGPT and LLMs mean for science?

- Change training ?
- Research integrity processes to change?
- Most LLMs are corporate proprietary products.
- Erroneous truth claims.
- Equity?
- Legal implications of LLMs for science?

AutoML to address skills needs?

Help bu

Will n
more

Research challenges could be organised around AutoML for science.

Research could be funded that involves applying AutoML in AI-driven science.

Knowledge without understanding ?

What if an AI finds something like this:

$$(x-2)^2(y-2x+2)^2(y+2x-10)^2(x-4)^2(y-2x+8)^2(y+2x-16)^2\left(y-3-3\left\lfloor x-\frac{11}{2}\right\rfloor^2\right)^2(x-8)^2$$

$$\cdot\left(y-2-3\left\lfloor\frac{x-8}{2}\right\rfloor^2\right)^2(x-11)^2\left(y-\frac{1}{2}x+\frac{5}{2}-3\left\lfloor\frac{x-11}{2}\right\rfloor^2\right)^2\left(y+\frac{1}{2}x-\frac{17}{2}-3\left\lfloor\frac{x-11}{2}\right\rfloor^2\right)^2(x-15)^2$$

$$\cdot\left(y-4-3\left\lfloor\frac{x-14}{2}\right\rfloor^2\right)^2(y-2x+52)^2(x-17)^2(y+x-21)^2(x-19)^2\left(y-x+17-3\lfloor x-20\rfloor^2\right)^2$$

$$\cdot\left(y+x-23-3\lfloor x-20\rfloor^2\right)^2\left(y-x+19-3\lfloor x-21\rfloor^2\right)^2\left(y-3-3\lfloor x-21\rfloor^2\right)^2(x-25)^2\left(y+\frac{1}{4}x-\frac{41}{4}-3\left\lfloor\frac{x-25}{2}\right\rfloor^2\right)^2$$

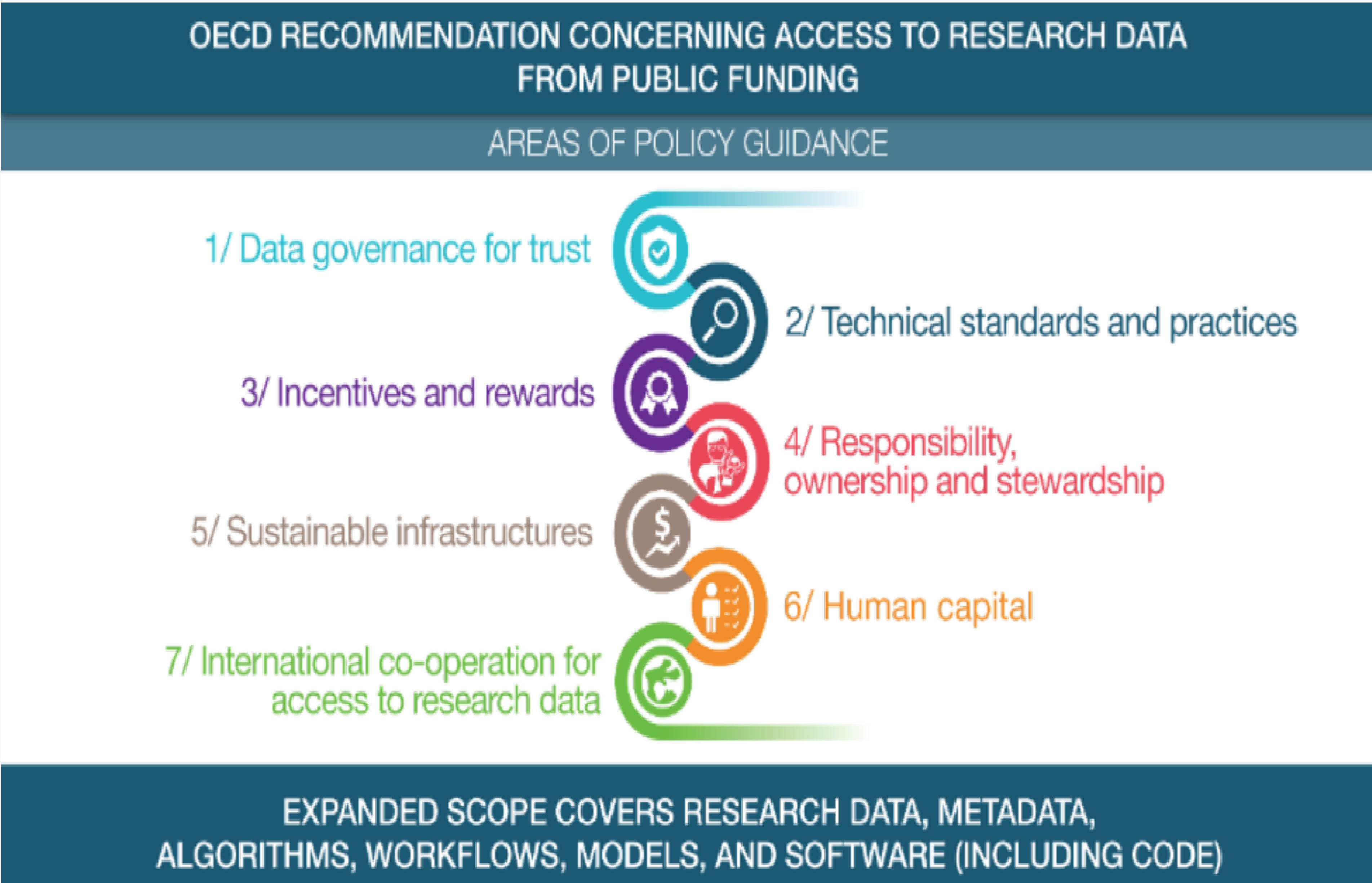
$$\cdot\left(y-\frac{1}{8}x-\frac{1}{8}-3\left\lfloor\frac{x-25}{2}\right\rfloor^2\right)^2\left(y+\frac{5}{8}x-\frac{151}{8}-3\left\lfloor\frac{x-25}{2}\right\rfloor^2\right)^2(y-2x+54)^2(y+2x-62)^2\left(y-3-3\left\lfloor x-\frac{57}{2}\right\rfloor^2\right)^2$$

$$\cdot(x-31)^2(y+x-35)^2(x-33)^2(x-34)^2\left(y+\frac{1}{2}x-21-3\left\lfloor\frac{x-34}{2}\right\rfloor^2\right)^2\left(y-\frac{1}{2}x+15-3\left\lfloor\frac{x-34}{2}\right\rfloor^2\right)^2$$

$$\cdot((x-38)^2+(y-3)^2-1)^2(x-40)^2(y+2x-84)^2(y-2x+80)^2(x-42)^2(x-43)^2\left(y-2-3\left\lfloor\frac{x-43}{2}\right\rfloor^2\right)^2$$

$$\cdot(y-3-|x-47|)^2((x-47)^2+(y-3+\sqrt{y^2-6y+9})^2)^2+\left(y^2-6y+8+\sqrt{y^4-12y^3+52y^2-96y+64}\right)^2=0$$

Data


OECD RECOMMENDATION CONCERNING ACCESS TO RESEARCH DATA FROM PUBLIC FUNDING
AREAS OF POLICY GUIDANCE
1/ Data governance for trust
2/ Technical standards and practices
3/ Incentives and rewards
4/ Responsibility, ownership and stewardship
5/ Sustainable infrastructures
6/ Human capital
7/ International co-operation for access to research data
EXPANDED SCOPE COVERS RESEARCH DATA, METADATA, ALGORITHMS, WORKFLOWS, MODELS, AND SOFTWARE (INCLUDING CODE)