

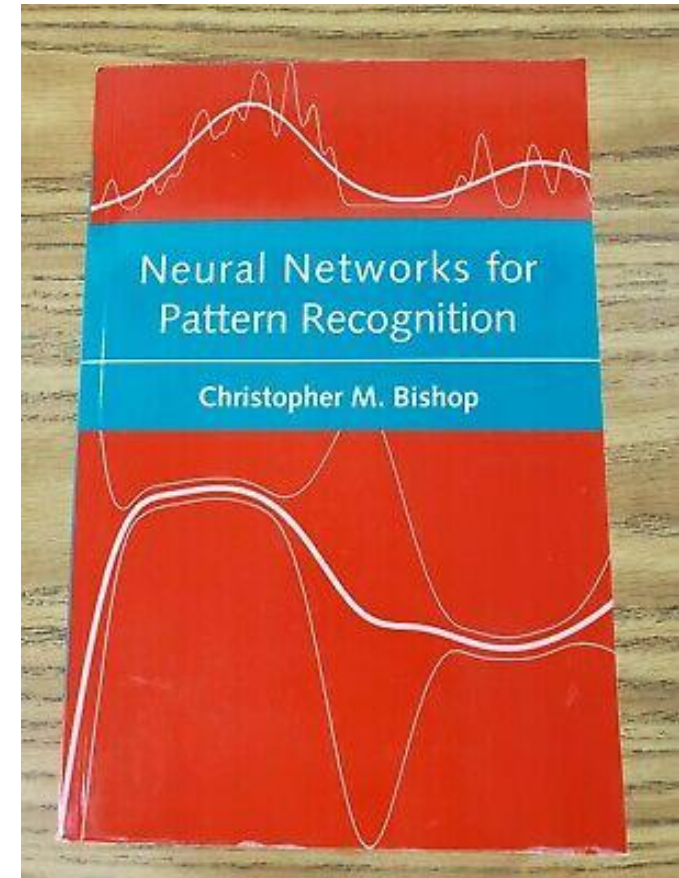
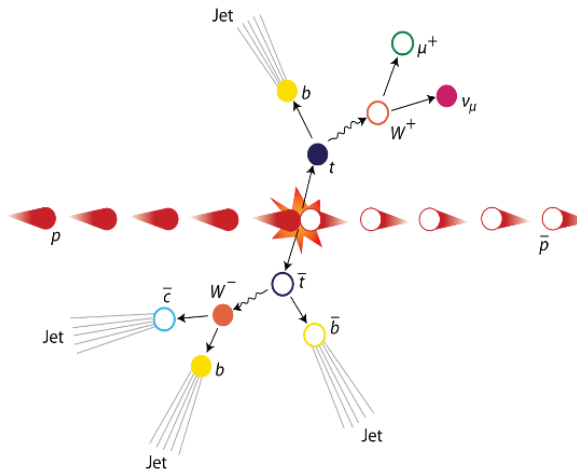
ARTIFICIAL INTELLIGENCE AND SCIENTIFIC ENDEAVOUR

BENEFITS AND CHALLENGES

AMOS STORKEY
SCHOOL OF INFORMATICS
UNIVERSITY OF EDINBURGH

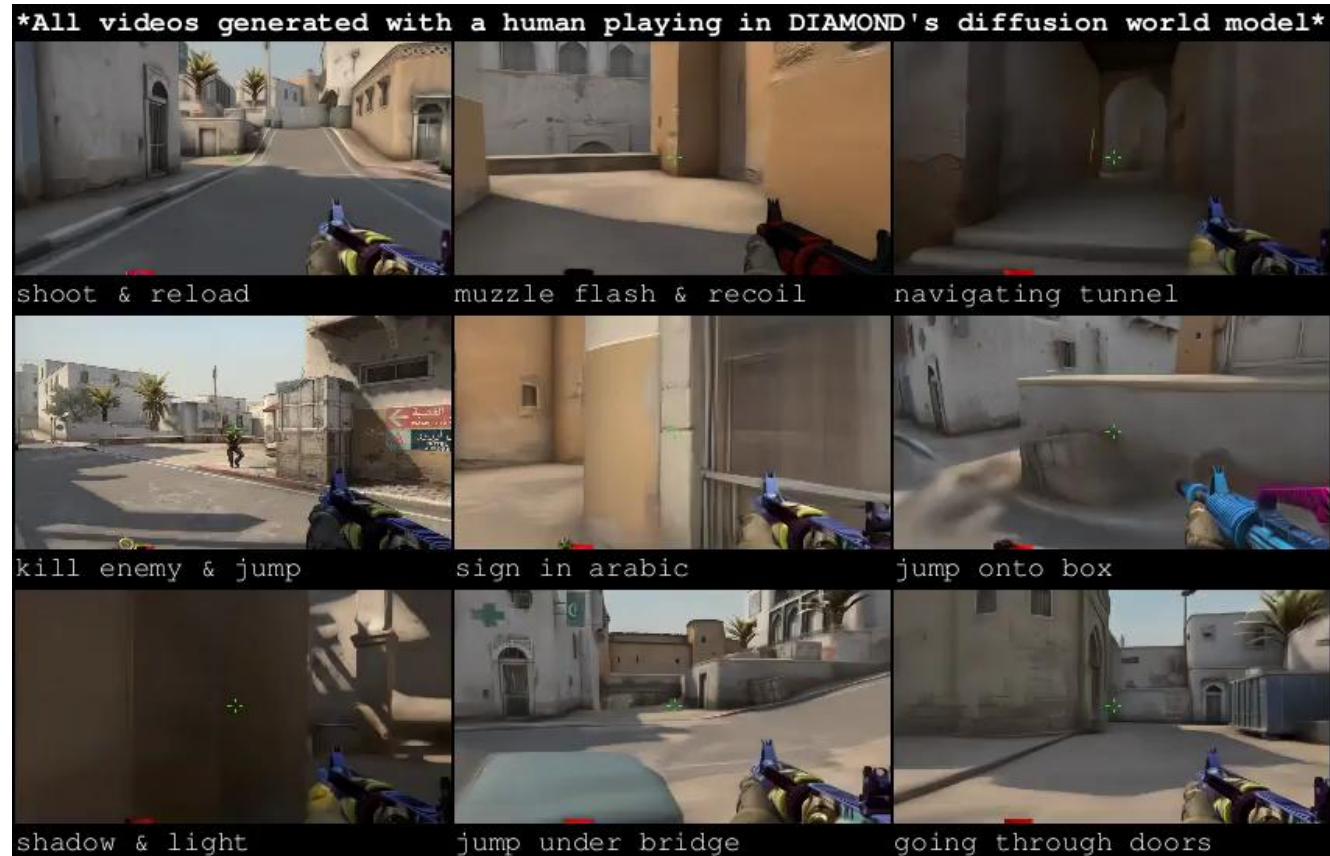


1995



AI TODAY?

- DIAMOND: <https://diamond-wm.github.io/>

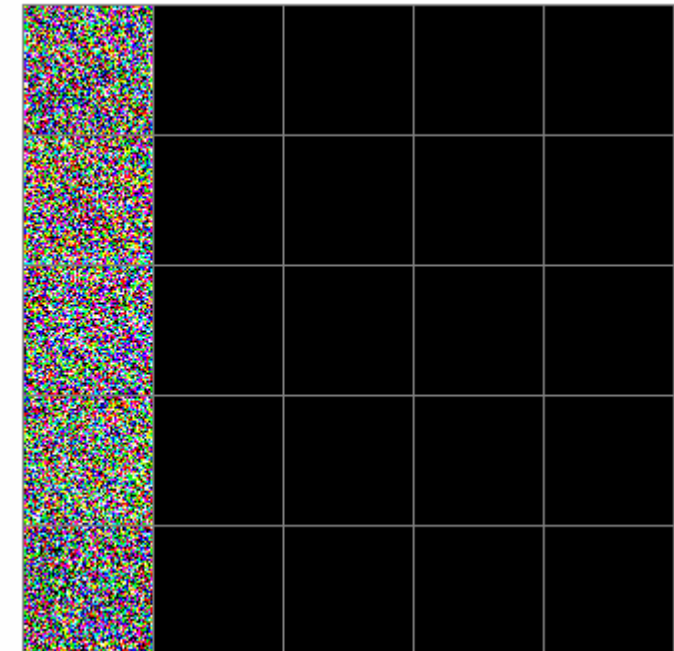


- Counterstrike Global Offensive. But does it understand geometry?
- Well yes... and no



Action

t=1



GENERALISATION AND GEOMETRY



THE PLAN

- AI and SCIENCE
- AI and SCIENTIFIC SOCIETY
- AI and the FUTURE

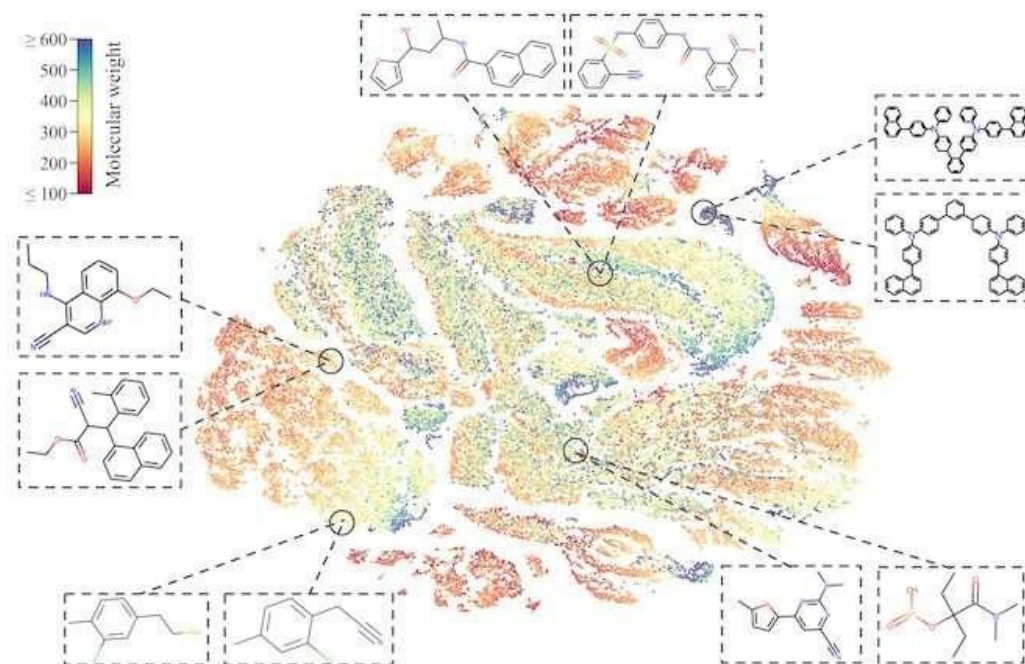


AI AND SCIENCE



AI, SCIENCE, AND MEDICINE

- **Physics:**
 - ◆ Emulators, Learning symmetries, finding Hamiltonian embeddings, detectors and analysers.
- **Chemistry:**
 - ◆ Molecular dynamics, molecular discovery, property prediction.
- **Biology:**
 - ◆ Systems biology, protein folding, modelling cellular growth and regeneration, computational neuroscience
- **Informatics:**
 - ◆ ML4Sys, language generation, programme discovery.
- **Geosciences:**
 - ◆ Weather systems, remote sensing, ice dynamics, ocean dynamics, digital twins.
- **Medicine:**
 - ◆ Drug discovery, predictive precision medicine, epidemiology, screening programmes.



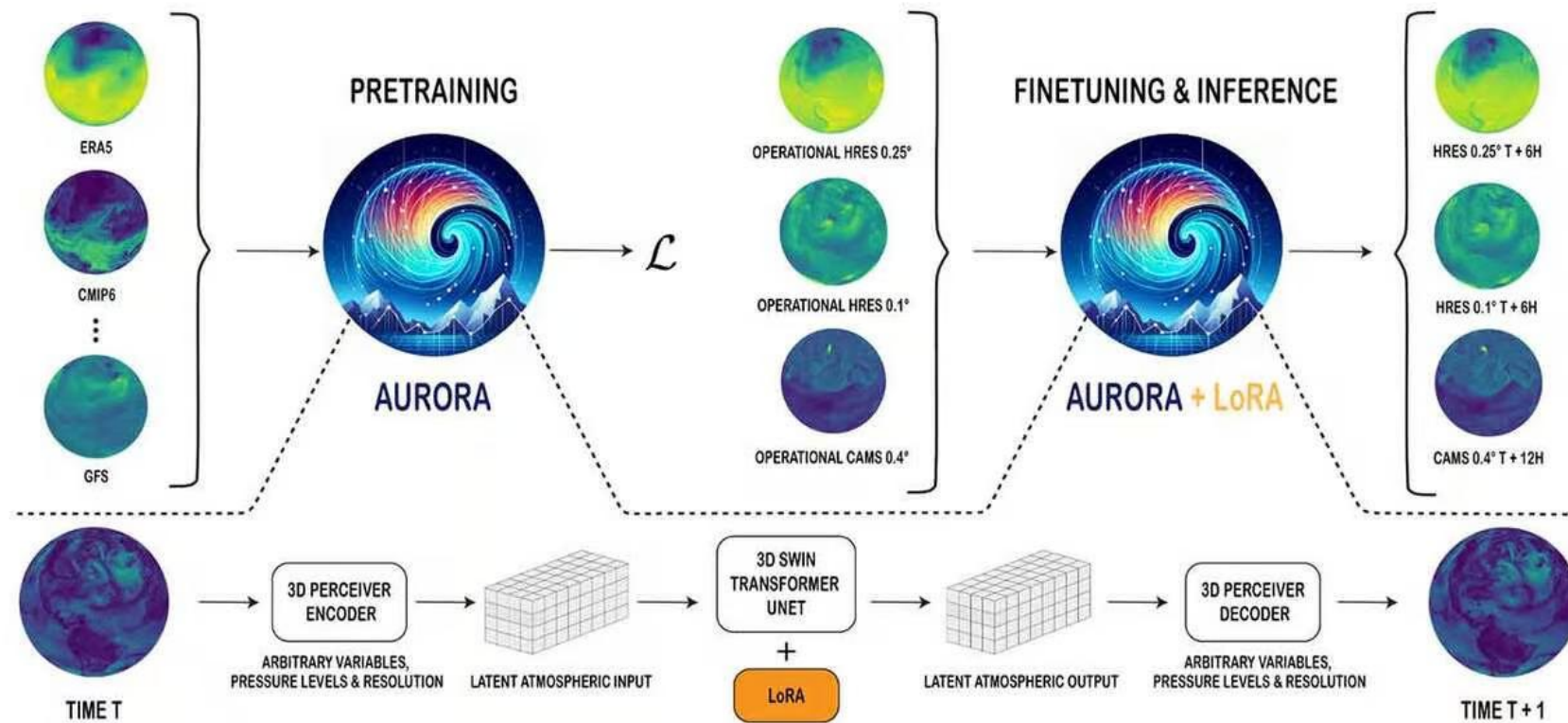
From Wang et al (2022) Molecular Contrastive Learning of Representations via Graph Neural Networks

Search, emulators, representation, generative models, risk, assimilation



EXAMPLE: AURORA

A flexible 3D foundation model of the atmosphere



From Bodnar et al (2024) [Aurora: A Foundation Model of the Atmosphere](#)



AI AND SCIENCE: THE CHALLENGES



Speed of change



Data ownership



Perceived value of
computation expertise



Privatization of science



Public AI engines?



Foundational AI v. AI applications?



Pay and value discrepancy



AI AND SCIENCE: SCIENTIFIC ACTIVITY

AI impacts science activity communication:

- Move beyond the paper model of scientific activity
- AI tools for planning, execution and evaluation: AI Assistants.
- Expansive models. But explainability? On human terms? Does that limit science?

Problems of the AI technology landscape

- Faking, cheating, deceptive use
- Variability collapse – lack of diverse thinking
- Control of small number of companies over thought
- Efficient tooling may reduce variance but increase bias
- Evaluation, understanding, interpretation



AI AND SCIENCE: SCIENTIFIC PROGRESS

- Lu et Al (2024) The AI Scientist: Towards Fully Automated Open-Ended Scientific Discovery. (Sakana AI – Nvidia backed)
- Future science will need AI tooling – like current science needs computation.
- **But** will there be a shift in what it means to “understand”? What is scientific knowledge? Whose knowledge?
- Human knowledge versus AI agent knowledge? Keeping the human in science?
- Making AI work for human scientific endeavour



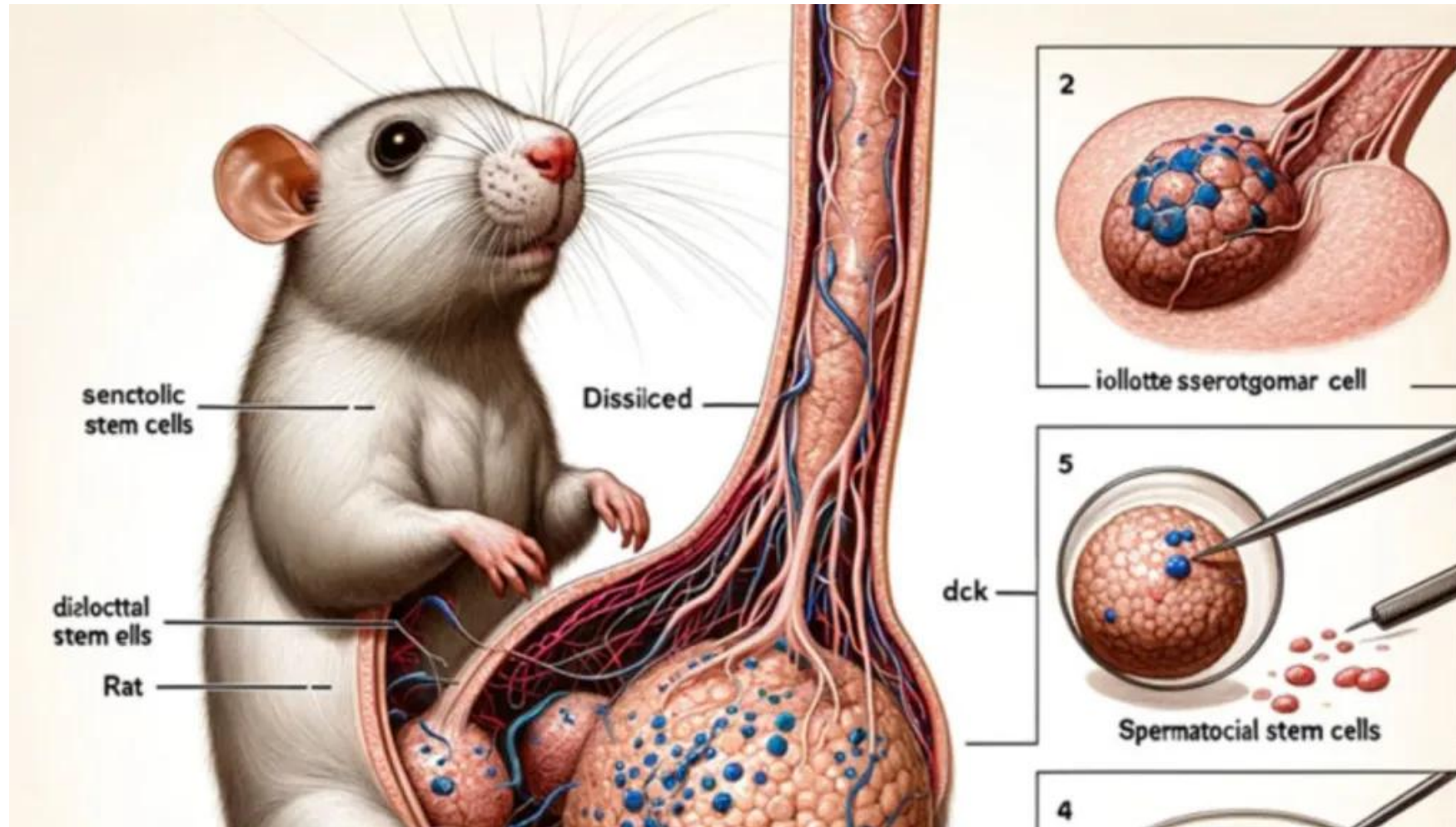
AI AND SCIENTIFIC SOCIETY



THE RAT



RETRACTION: THE OVER-ENDOWED RAT



AI AND SOCIETY: AUTOMATION

- AI, automation, deception, control.
- Large language models etc. are cheap and effective. Likely they:
 - ◆ Will further find their way into the writing of papers and proposals
 - ◆ Will further find their way into reviewing of papers and proposals
 - ◆ Will further direct the scientific enterprise towards AI-easy activity
 - ◆ Will replace humans at various points of the science process
- But they also are / will be:
 - ◆ Used to spam journals and conferences with fake papers
 - ◆ Used to create review and editor rings, fake reviewers etc.
 - ◆ Be easily leveraged or gamed to favour more powerful manipulative players
 - ◆ Reduce human-to-human interaction in scientific endeavour



AI AND SOCIETY: FIRMS AND LARGE MULTINATIONALS

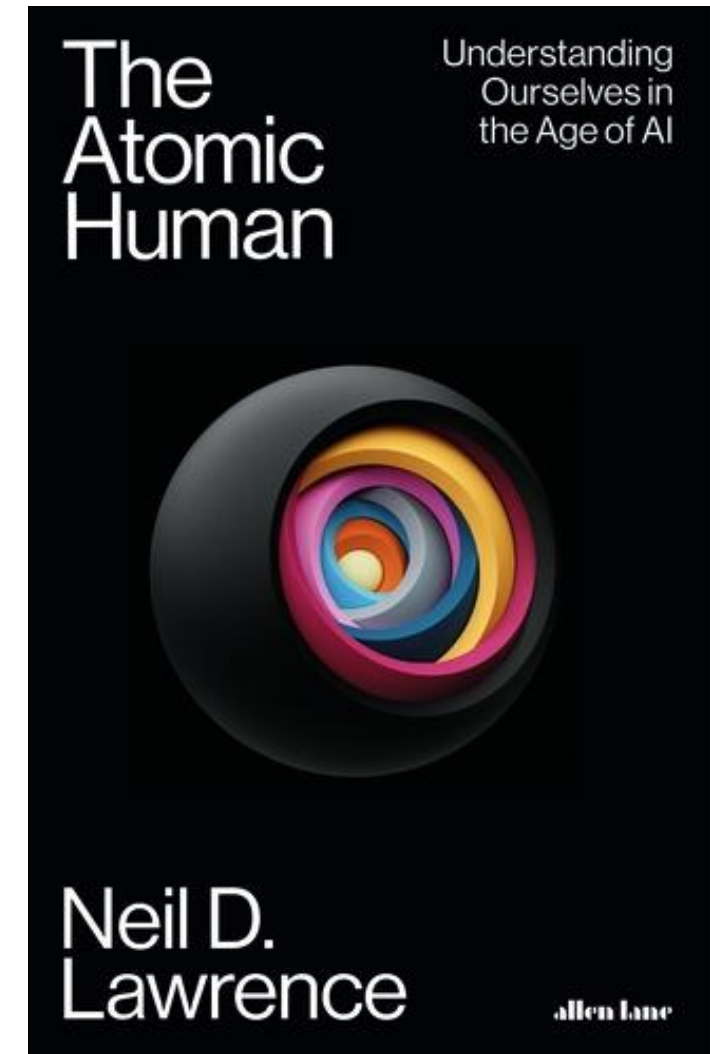
- The firm: an organism more powerful and more capable than individual humans
- Current: humans symbiotic in companies. Human workers, human owners, human customers
- Direction of travel: large internet companies built around automation.
 - ◆ Business scaling not about employees
 - ◆ High level of control of human capital
 - ◆ High economic control – “reinvest” rather than dividend
 - ◆ Finger in every pie. Including science.
- Future: B2B market growing massively compared with B2C market
- Potential for human-out-of-the-loop corporate environments dictating economy



ARTIFICIAL GENERAL INTELLIGENCE?

■ Careful:

- ◆ Concept of AGI is dubious. Concept of intelligence is dubious. Not one thing
- ◆ Neil Lawrence: the idea of AGI is a re-emergence of eugenic thinking. Need to know what it means to be human.
- ◆ But impact from AI and automation doesn't require "intelligence". It simply requires acquiescence.
- ◆ We have given power to automation, process, organisations for centuries.
- ◆ We, the people, choose to.



AI AND THE FUTURE

- Making AI work for people; making science work for people
- Making AI work for human scientific endeavour
- Companies are not necessarily on our side...
- Centralised data-assimilating AI?
- Or a distributed human-centric AI in Science? Human-aiding tooling, locally controlled, with use informed by knowledgeable users.



AI AND EUROPE

- What should European AI look like?
- Not competing at the large-internet-company monolithic-AI game.
- Something else – a distributed AI infrastructure at the edge.
- An AI economy of small lean communicating but distributed AI agents.
- In science – we want people to adapt and mould AI to aid their scientific curiosity. The way they see it. Not the way they are told to see it.



AI AND US: GOING FORWARD REALISTICALLY

- What should we embrace, what should we guard against, what should we change? And how?
- How do we harness the good? Resourcing, emphasis, engagement, collaboration
- The power and futility of regulation.
- Technological defences.
- The power of education?
- Emphasis on science as human endeavour not disembodied knowledge?
- Distributed collaborative edge AI: AI in the control of people not companies?
- Data ownership, data sharing.



BREAKOUT

■ REPORTS:

- ◆ International Science Council
<https://council.science/news/ai-in-science/>
- ◆ Royal Society
<https://royalsociety.org/news-resources/projects/science-in-the-age-of-ai/>

■ QUESTIONS and ACTIONS:

- ◆ How do we protect the scientific endeavour from the more dubious AI scams?
- ◆ How do we change the funding, collaboration and reviewing landscape to enable the right kind of AI advances?
- ◆ How to we ensure that automation and AI enhances human inquisitiveness and drive for understanding?
- ◆ How do we avoid a dominance of a few large agents (e.g. large multinationals) in determining our Scientific directions?
- ◆ What sort of AI research helps to empower people rather than reduce them?
- ◆ How do we build better collaborations between Scientists and AI researchers?
- ◆ How should we view large companies trying to dominate in control over AI?
- ◆ How do we enable a European AI strength and agenda?
- ◆ What is our vision and hope for what Science should look like in 15 years time? And AI?

