



**TÉCNICO**  
LISBOA

# **IA and Scientific Research**

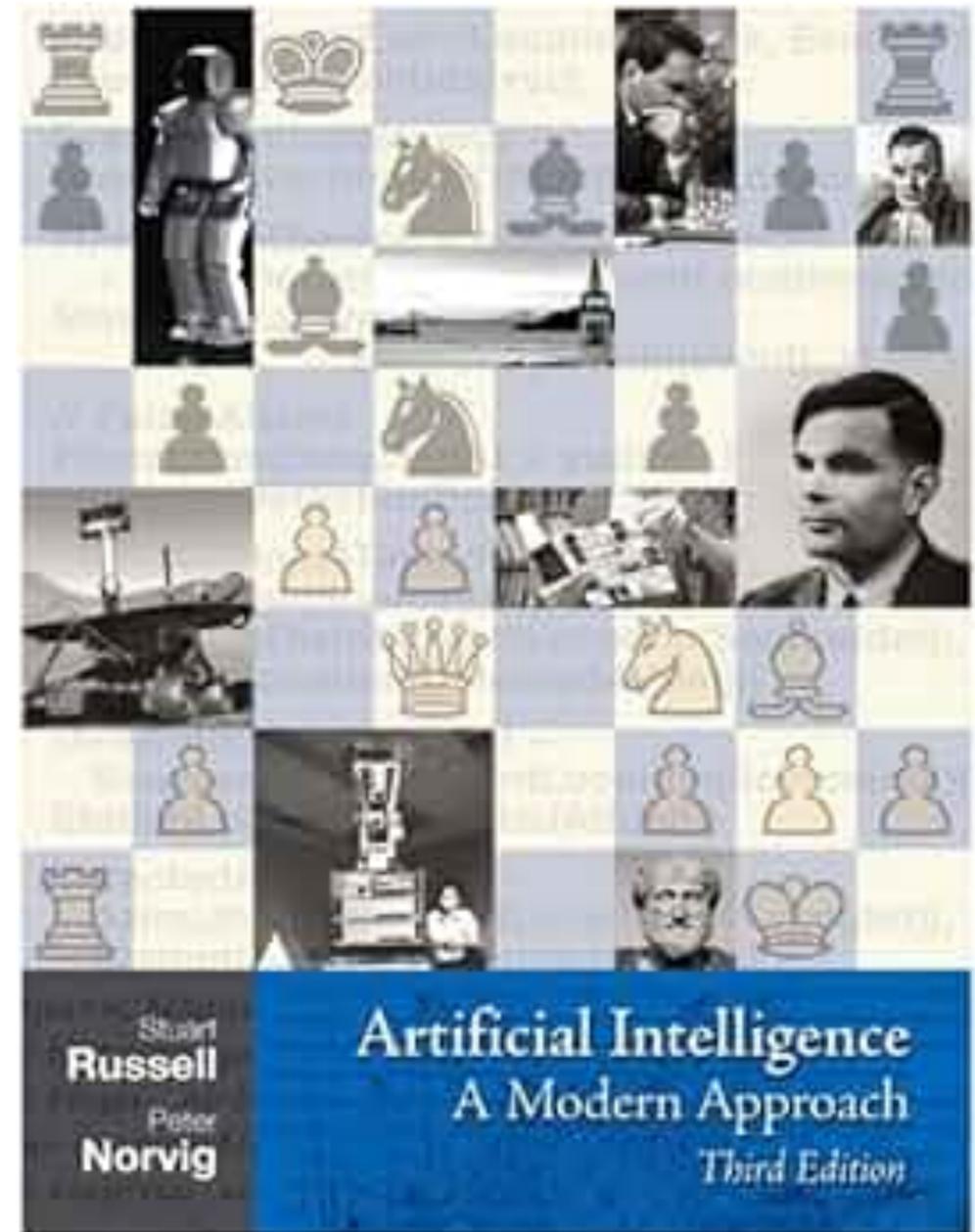
Francisco S. Melo

**Shaping the Future 2024**

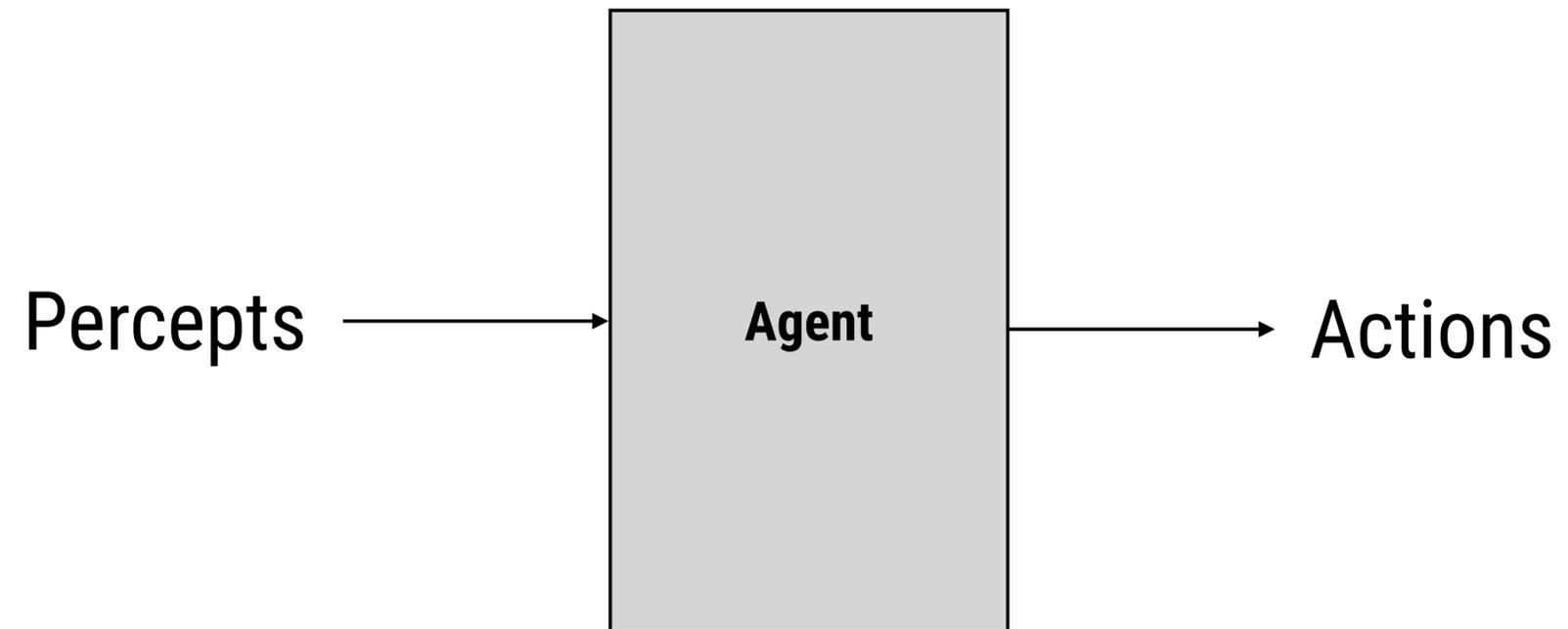
# What is AI?

*“The study of [intelligent] agents that receive precepts from the environment and take actions. Each such agent is implemented by a function that maps percepts to actions [...].”*

Russel & Norvig, 2010



# What is AI?



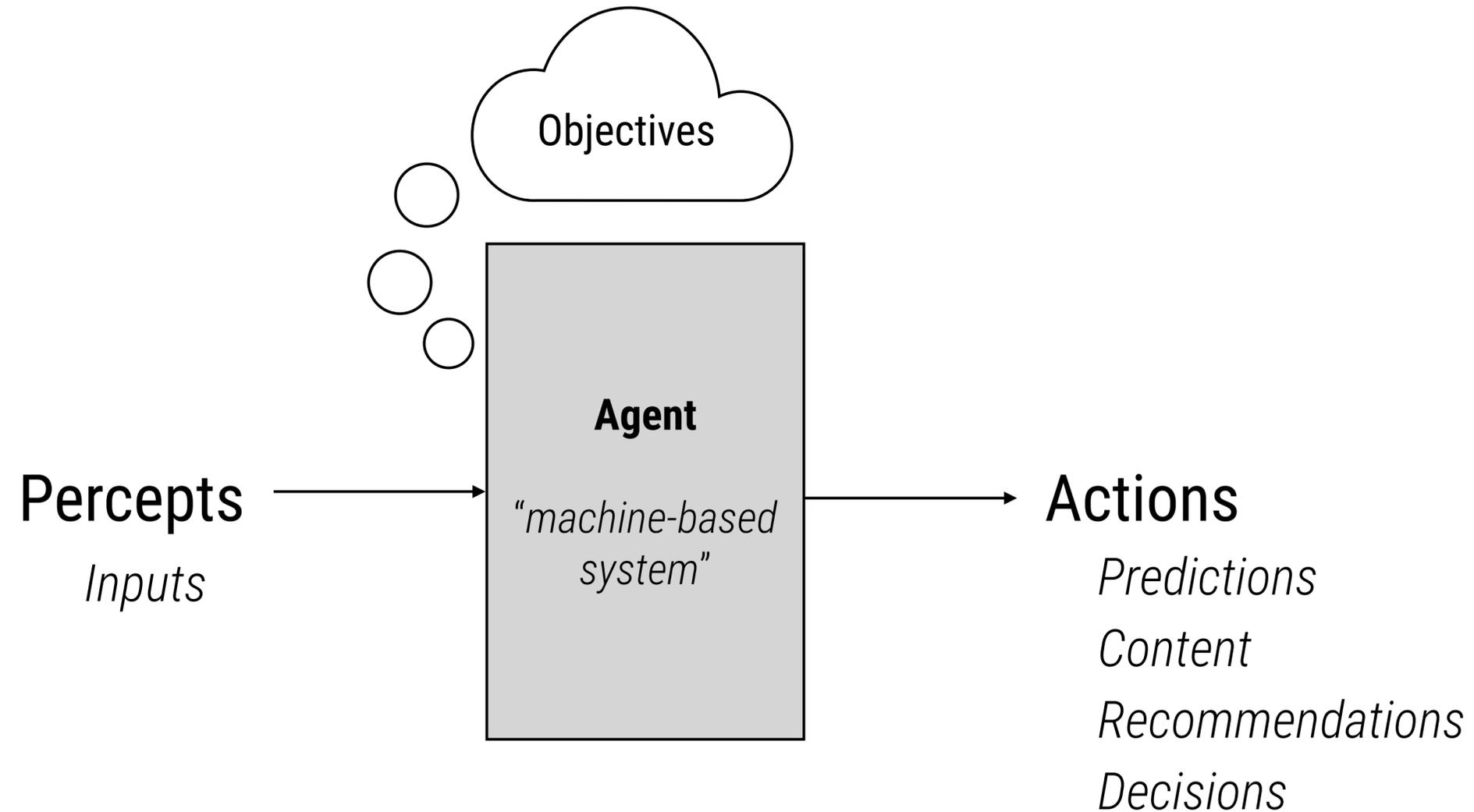
# What is AI?

*“A machine-based system designed to operate with varying levels of autonomy and that may exhibit adaptiveness after deployment and that, for explicit or implicit objectives, infers, from the input it receives, how to generate outputs such as predictions, content, recommendations, or decisions that can influence physical or virtual environments.”*

EU AI Act



# What is AI?

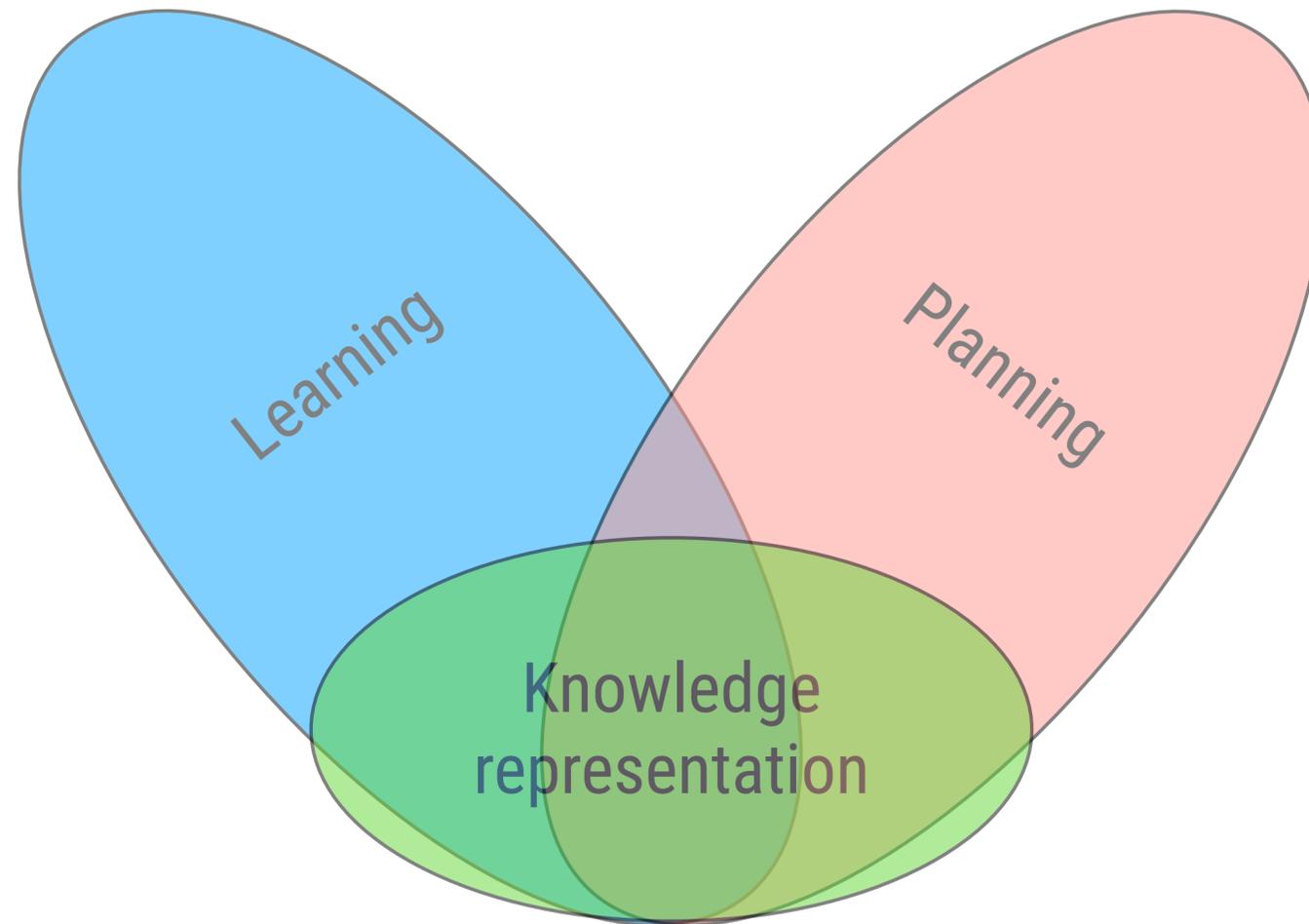


# Different schools of thought

Research in AI as...

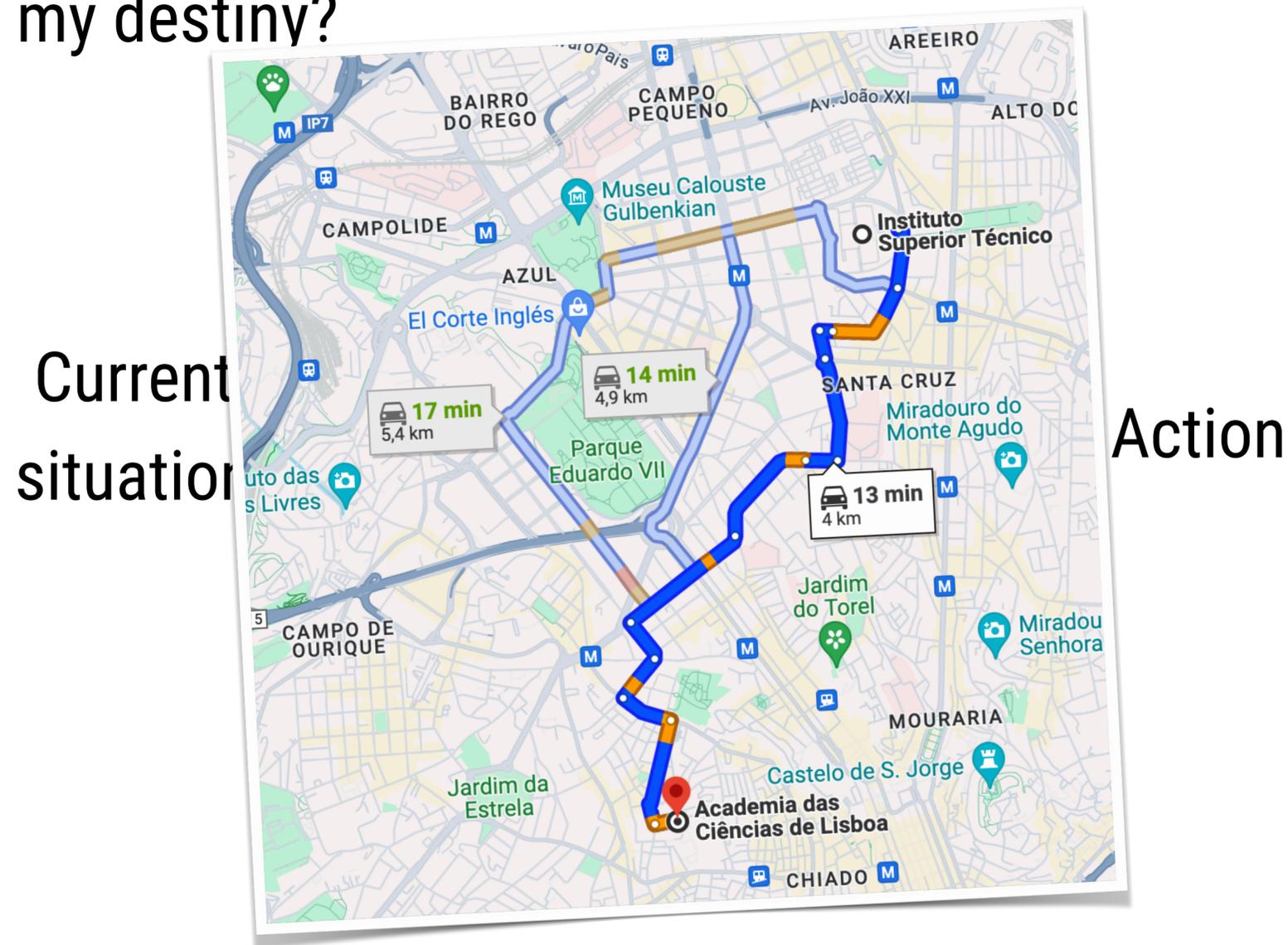
- ... building models (“machines”) that think **like humans**
- ... building models (“machines”) that act **like humans**
- ... building models (“machines”) that act **rationally**
- ... building models (“machines”) that think **rationally**

# Two heads of AI



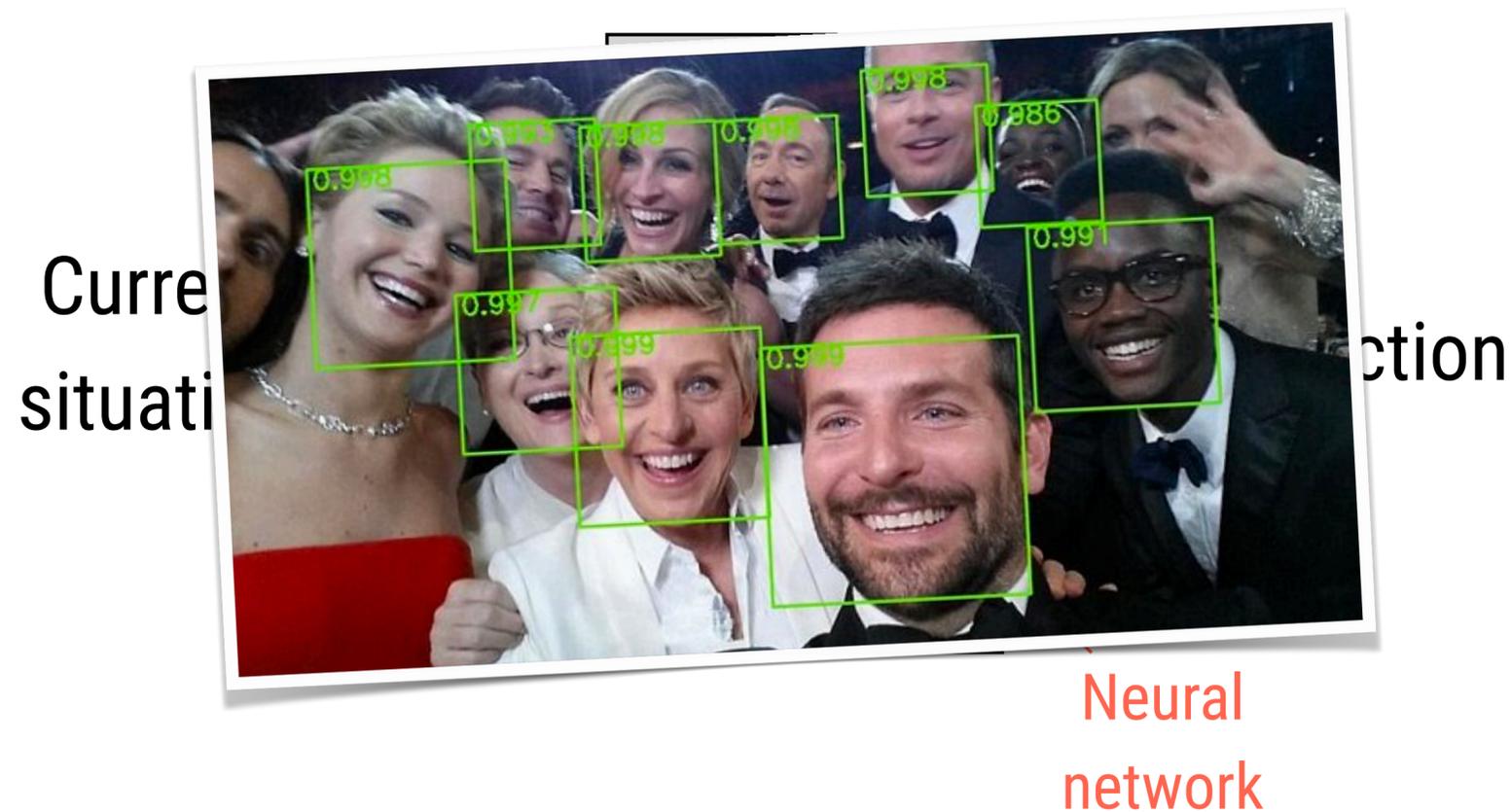
# Two heads of AI

- **Planning:** Given the current situation, what is the best action (sequence of actions) that takes me to my destiny?



# Two heads of AI

- **Learning:** How to use experience to improve my performance in my current task (in terms of action choice)?



# Why all the fuss?

**Microsoft's new breakthrough: AI that's as good as humans at listening... on the phone**

Microsoft's new speech-recognition record means professional transcribers could be among the first to lose their jobs to artificial intelligence.



Written by **Liam Tung**,  
Contributor

on October 19, 2016 | Topic: Innovation

# Why all the fuss?

## Google unleashes deep learning tech on language with Neural Machine Translation

Devin Coldewey @techcrunch / 9:14 PM GMT+1 • September 27, 2016

 Comment

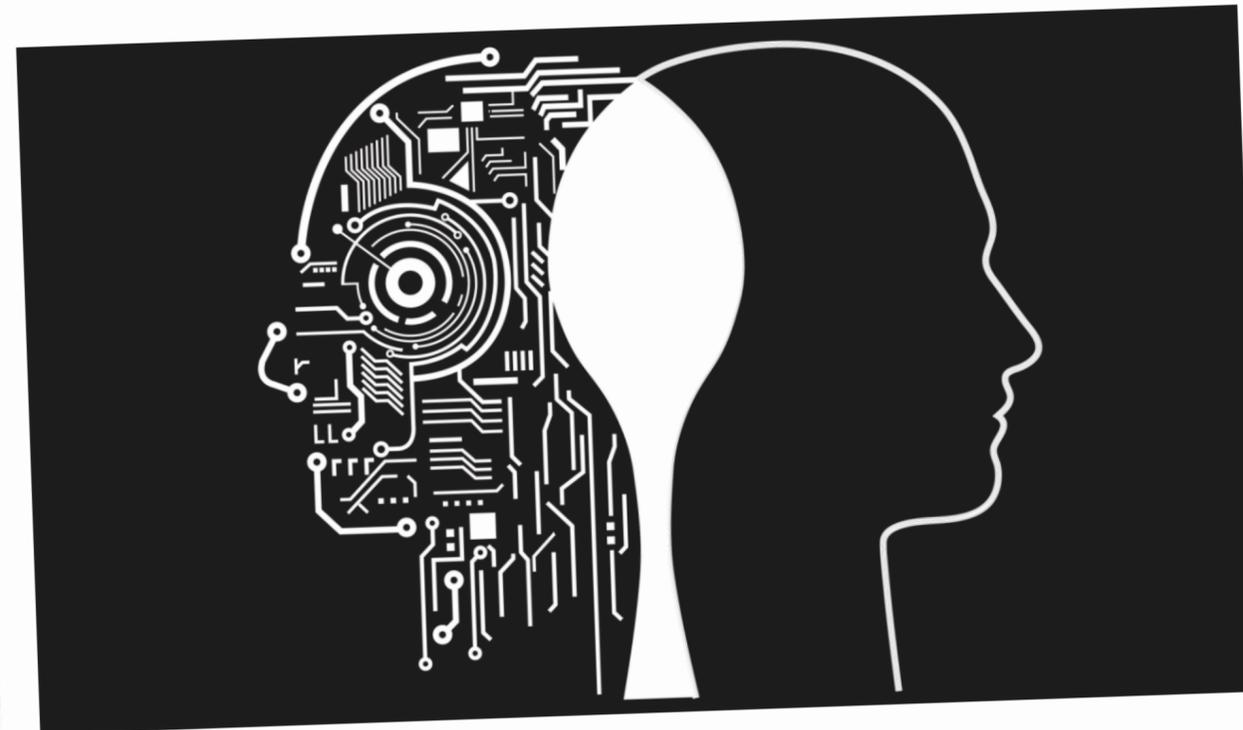


 Image Credits: razum / Shutterstock

Translating from one language to another is hard, and creating a system that does it automatically is a major challenge, partly because there are just so many words, phrases and rules to deal with. Fortunately, neural networks eat big, complicated data sets for breakfast.

# Why all the fuss?

A robot wrote this entire article. Are you scared yet, human?

*GPT-3*

We asked GPT-3, OpenAI's powerful new language generator, to write an essay for us from scratch. The assignment? To convince us robots come in peace

- For more about GPT-3 and how this essay was written and edited, please read our editor's note below



# Why all the fuss?



## Dall-E 2: Why the AI image generator is a revolutionary invention

By [Alex Hughes](#) Published: 06th May, 2022 at 09:25

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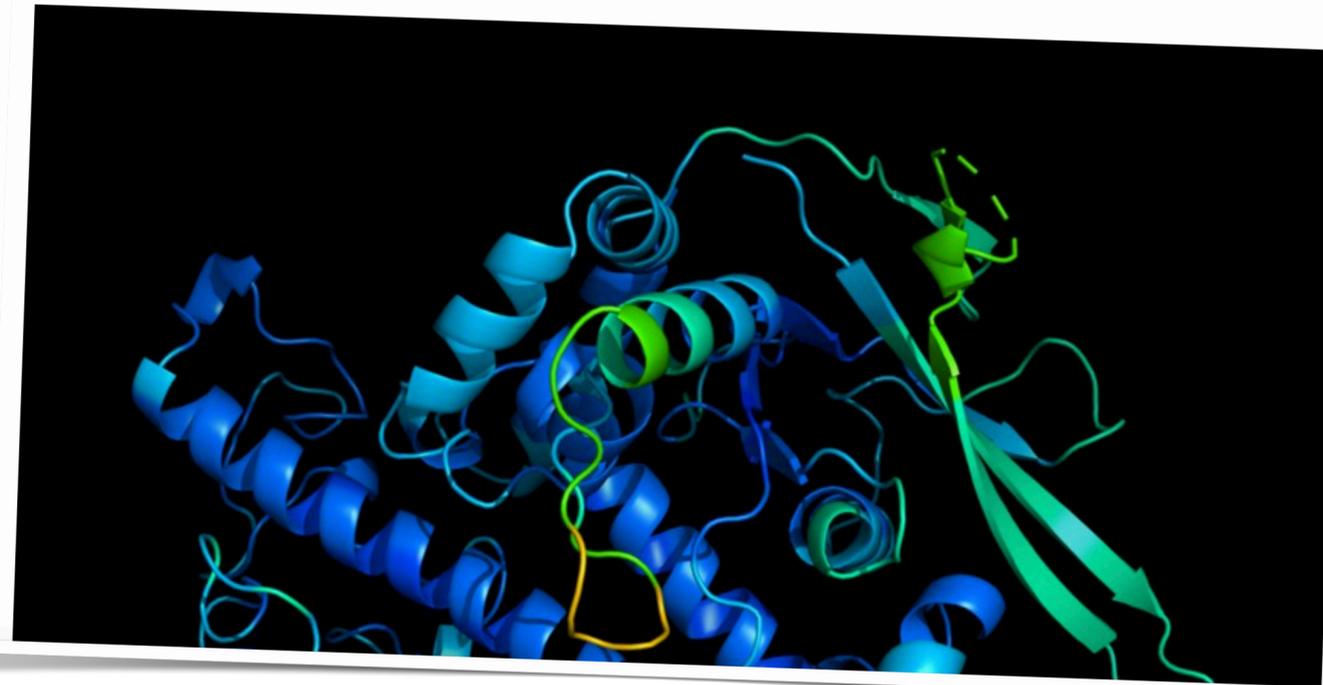
A piece of software is able to generate detailed images from just a short,

# Why all the fuss?

## **'It will change everything': DeepMind's AI makes gigantic leap in solving protein structures**

Google's deep-learning program for determining the 3D shapes of proteins stands to transform biology, say scientists.

[Ewen Callaway](#)



# Why all the fuss?

## This New AI Algorithm Can Master Games Without Being Told The Rules

BY SHRADDHA GOLED



# Why all the fuss?

## DeepMind's StarCraft-playing AI beats 99.8 per cent of human gamers



TECHNOLOGY 30 October 2019

By [Donna Lu](#)

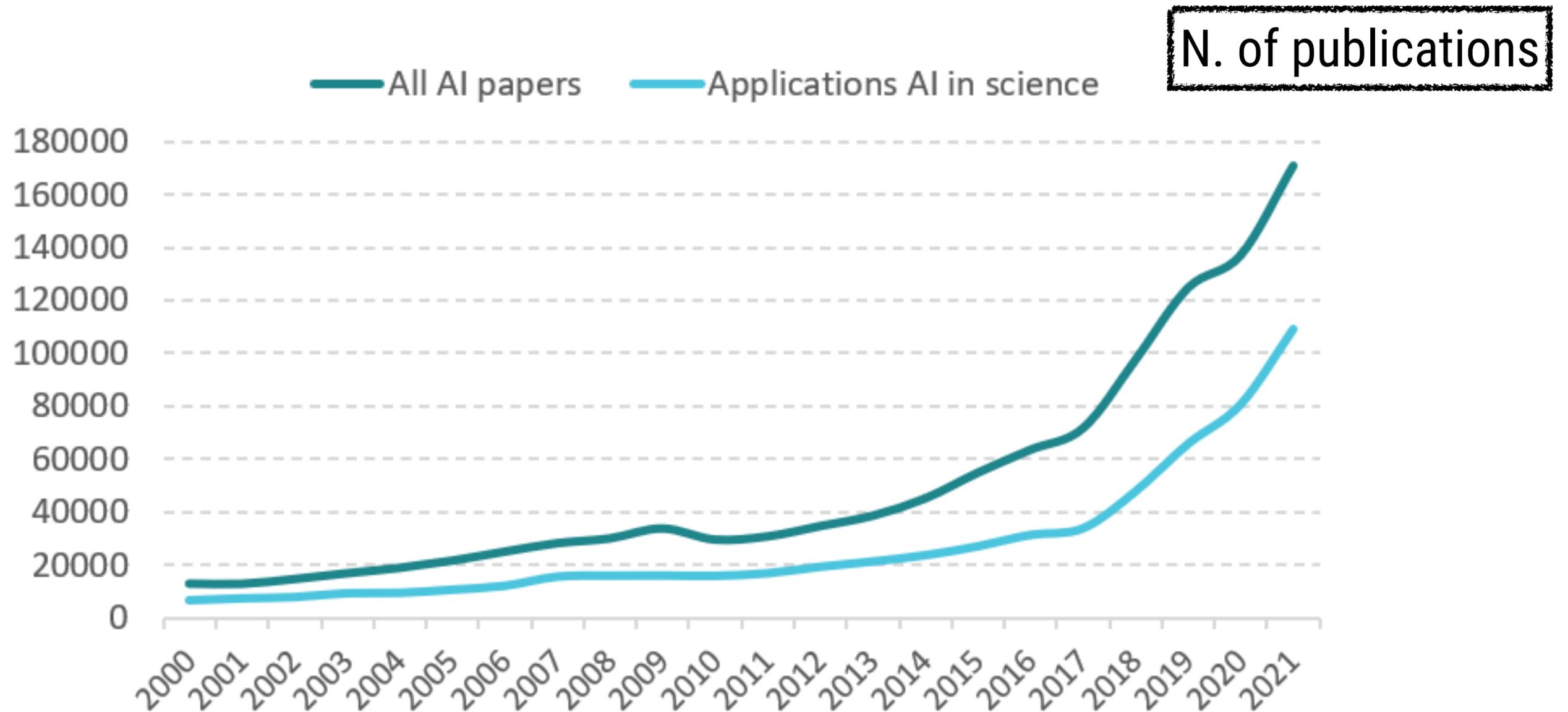


# Why all the fuss?



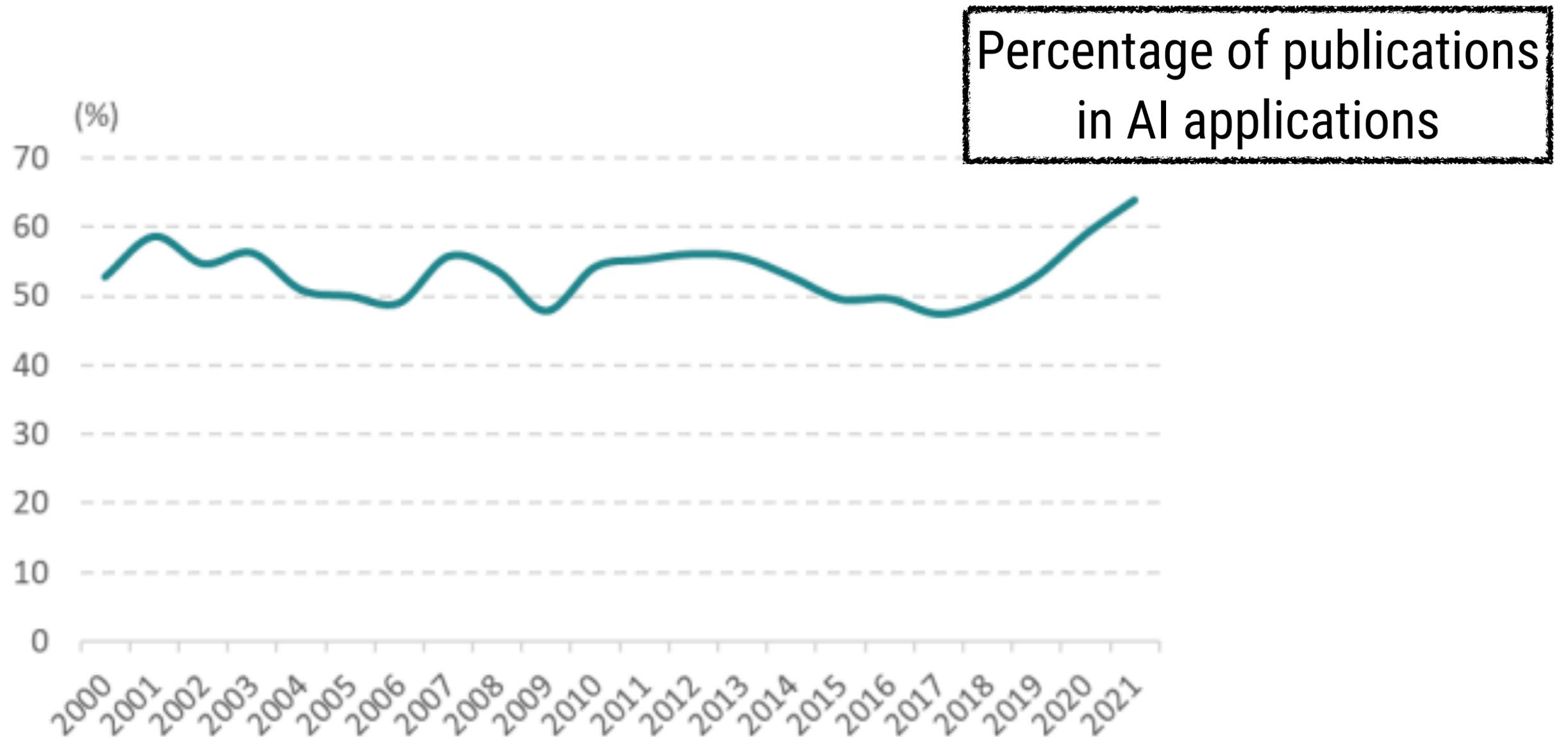
Source: European Commission, DG in R & D. Computation using Web of Science data.  
Annual growth computed as a 3-year rolling average.

# Why all the fuss?



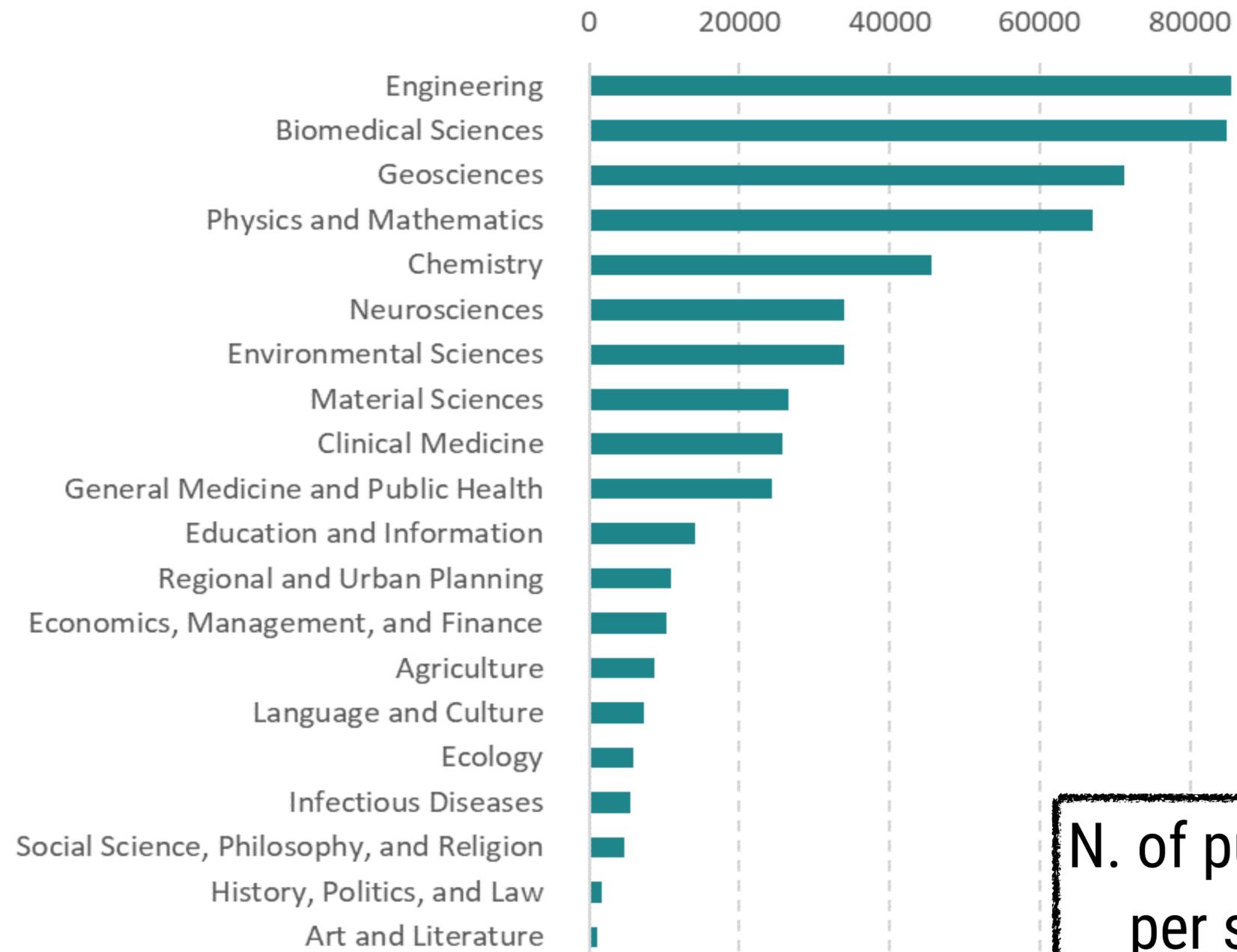
Source: European Commission, DG in R & D. Computation using Web of Science data

# Why all the fuss?



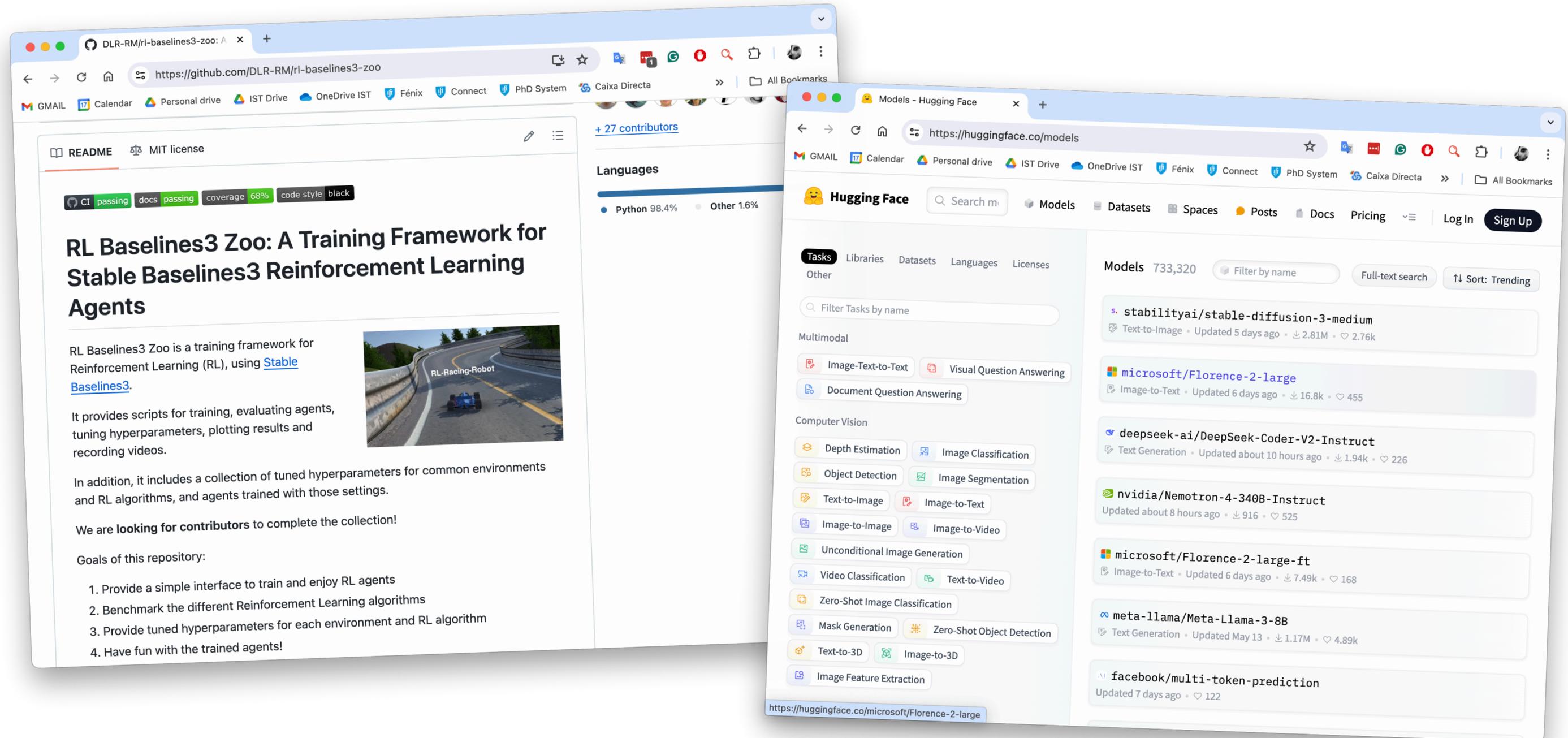
Source: European Commission, DG in R & D. Computation using Web of Science data

# IA and different disciplines



N. of publications in AI  
per scientific area

# AI for everyone



# AI for everyone

model.  
Furthermore, we will evaluate any setting of the neural network's parameters using a loss function. We'll examine its probability distributions and use the labels, which are essentially the identities of the next character. Gradient-based optimization will then be employed to adjust the network's parameters, ensuring the neural network accurately predicts the next character.

First step is to create a training set of all the bigrams for the model

### Create Bigram dataset for neural network

Create a training set of bigrams (x, y). Given the first character of Bigram, we try to predict the next character. 'xs' holds numerical representation of names characters. While 'ys' are targets/labels.

```
# Create training set of bigrams (x,y).  
# Given the first character of Bigram, we try to predict the next character.  
xs, ys = [], []  
for w in words:  
    chs = ['.'] + list(w) + ['.']  
    for ch1, ch2 in zip(chs, chs[1:]):  
        xs.append(stoi[ch1])  
        ys.append(stoi[ch2])  
xs = torch.tensor(xs)  
ys = torch.tensor(ys)  
print(words[:2])  
print(f'xs: {xs[:12]}')  
print(f'ys: {ys[:12]}')  
"""  
['emma', 'olivia']  
tensor([ 0,  5, 13, 13,  1,  0, 15, 12,  9, 22,  9,  1])  
tensor([ 5, 13, 13,  1,  0, 15, 12,  9, 22,  9,  1,  0])  
"""
```

### Feeding integers into neural network? One-hot encoding

How to feed these examples into the neural network? The integer values (like 1 for 'A', 2 for 'B', etc.), can imply a certain ordinal relationship or magnitude that doesn't actually exist in the context of language. For instance, the model might incorrectly interpret that 'B' (2) is twice as much as 'A' (1) or that 'C' (3)

## Build your own Transformer from scratch using Pytorch

Building a Transformer model step by step in Pytorch

Arjun Sarkar · Follow  
Published in Towards Data Science · 7 min read · Apr 26, 2023

678 12

Figure 1. Photo by Kevin Ku on Unsplash

In this tutorial, we will build a basic Transformer model from scratch using PyTorch. The Transformer model, introduced by Vaswani et al. in the paper "Attention is All You Need," is a deep learning architecture designed for sequence-to-sequence tasks, such as machine translation and text summarization. It is based on self-attention mechanisms and has become the foundation for many state-of-the-art natural language processing

## Mastering Atari Game: Deep Q-Network (DQN) Agents in Reinforcement Learning

Kabila MD Musa · Follow  
7 min read · Oct 15, 2023

8

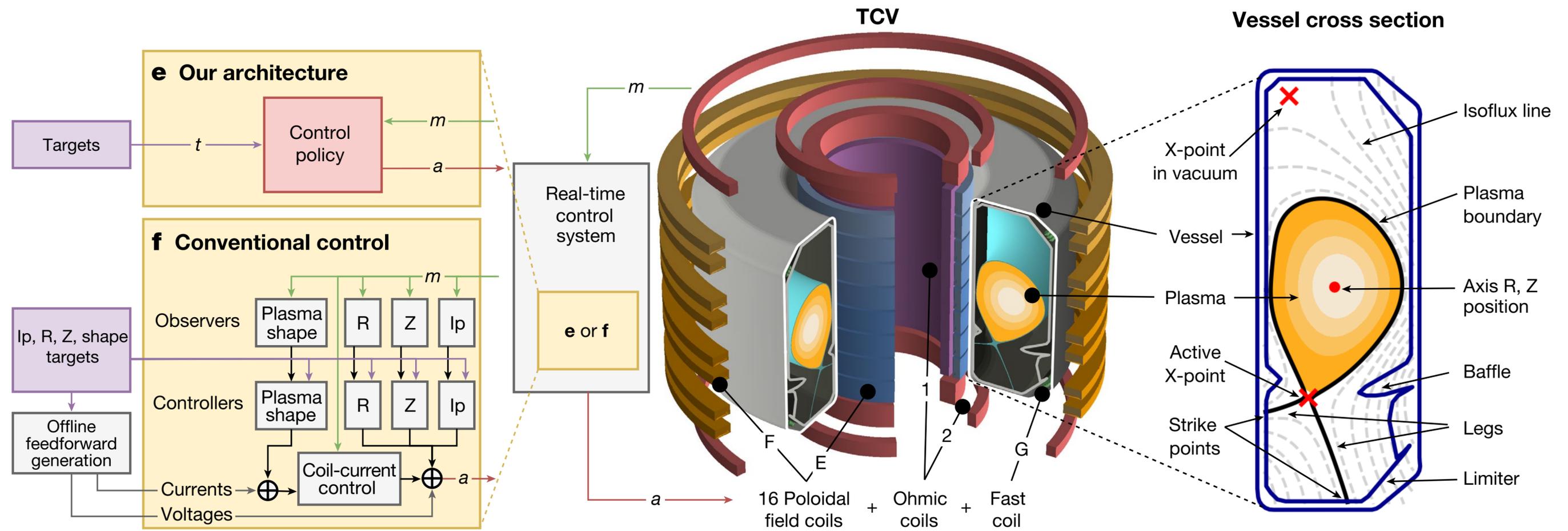
Photo by ELLA.DQN on Unsplash

Reinforcement Learning (RL) is a subfield of machine learning where an agent learns to make sequential decisions by interacting with an environment. One of the popular techniques in RL is the Deep Q-Network (DQN), which combines Q-learning with deep neural networks to tackle complex decision-making problems. In this blog post, we will explore DQN agents implemented in three different OpenAI Gym environments: CartPole, Space Invaders, and Pacman.

# Success stories

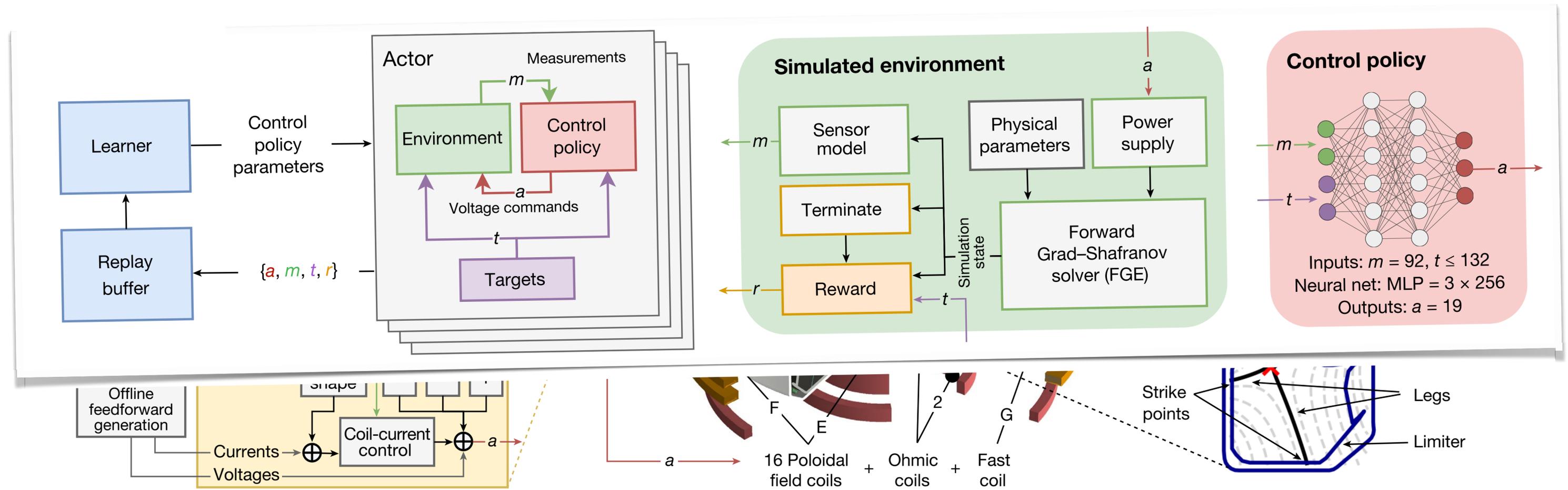
# Tokamak

- Delgrave et al (2022) proposed a novel approach, based on **reinforcement learning**, to optimize the magnetic control of tokamak



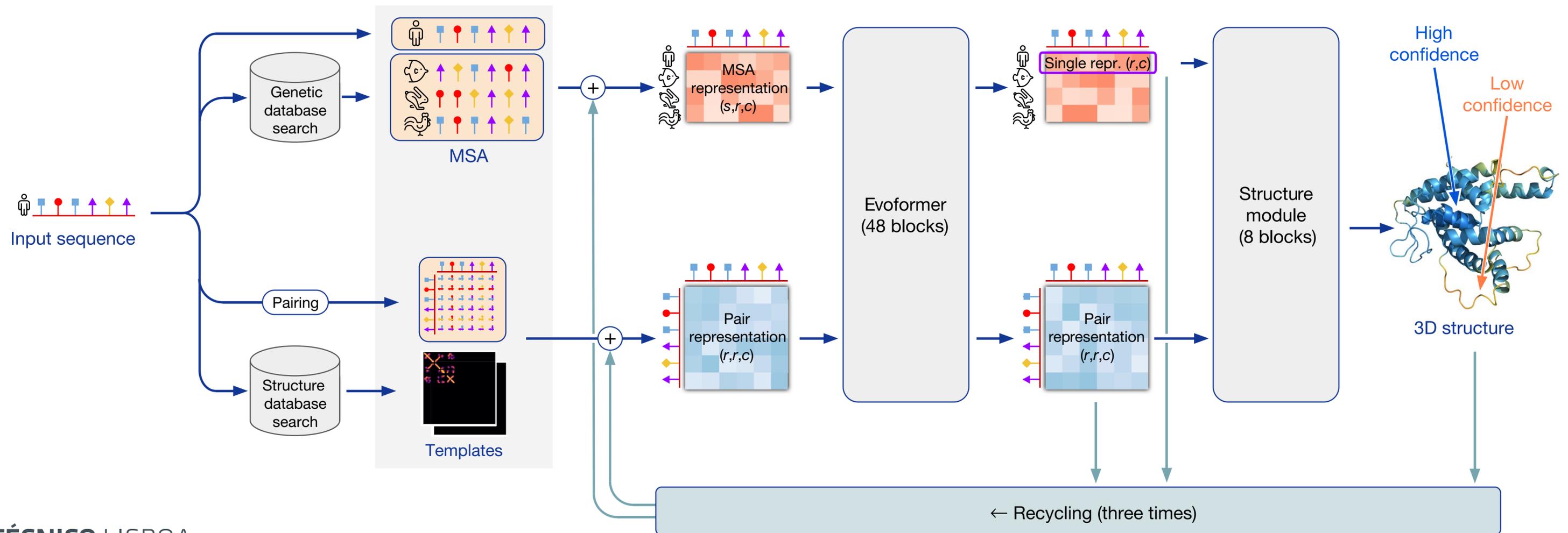
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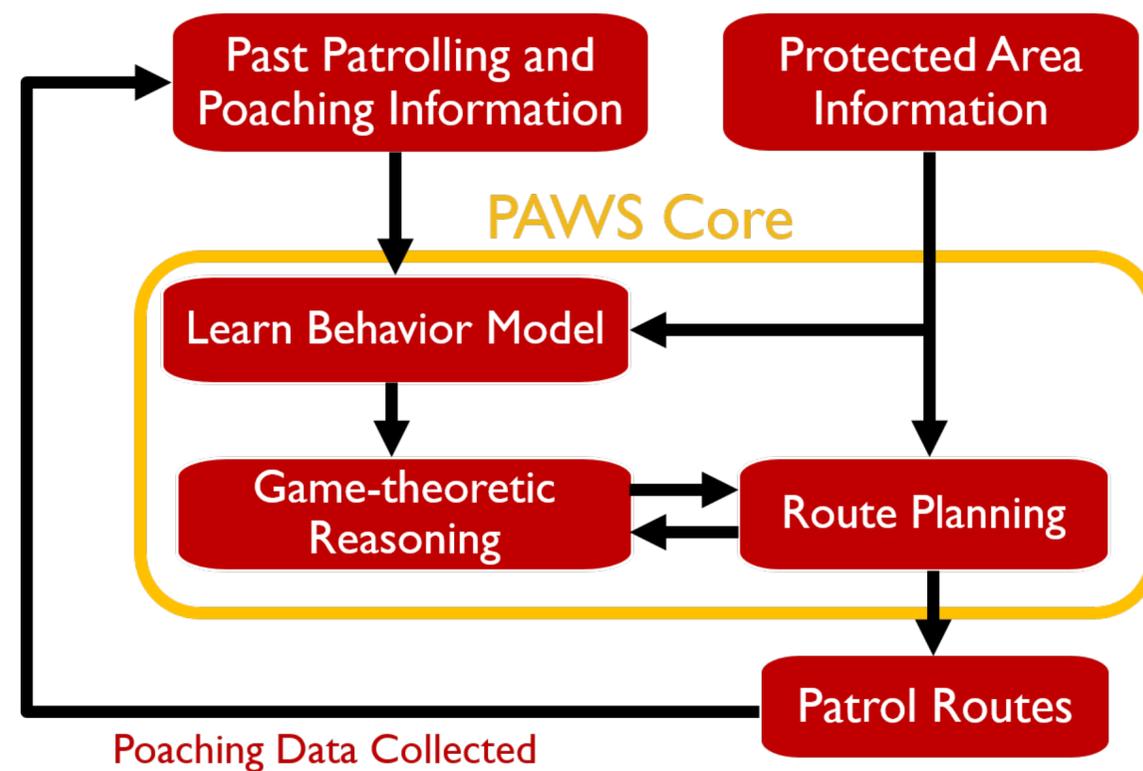
# AlphaFold

- Jumper et al (2021) proposed a new neural network architecture that - given a protein's aminoacid sequence - predicts the 3D structure of that protein



# Wildlife preservation

- Tambe et al (Xu et al, 2022) developed the PAWS system (Protection Assistant for Wildlife Security)



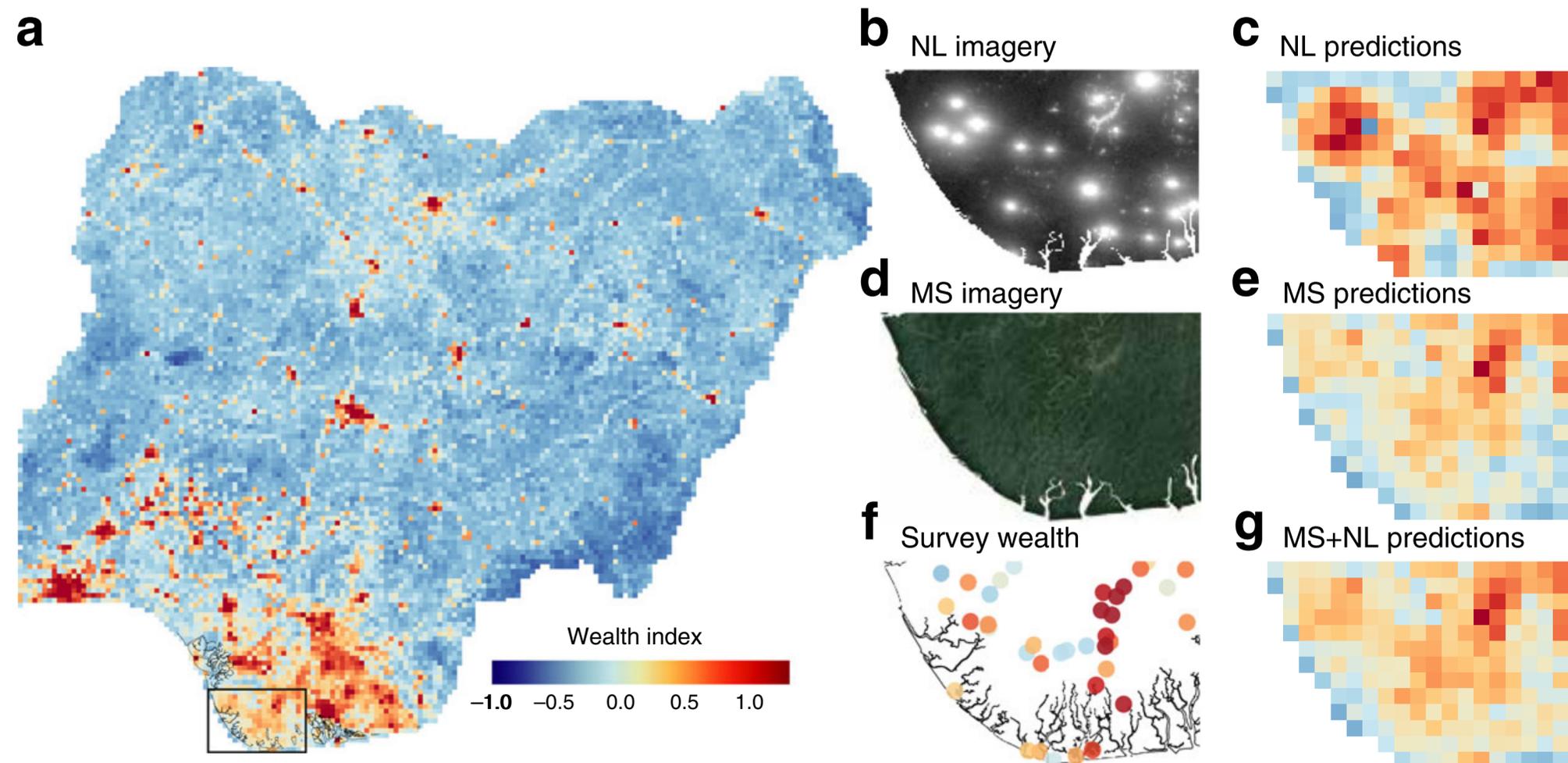
# Wildlife preservation

- Tambe et al (Xu et al, 2022) developed the PAWS system (Protection Assistant for Wildlife Security)
- PAWS allows forest rangers to optimize their patrols to maximize the probability of finding snares and other traps



# Fighting poverty

- Ermon et al (2020) used publicly available satellite images to - using the amount of nightlight - predict the levels of poverty in different countries in África



**“What about my research?”**

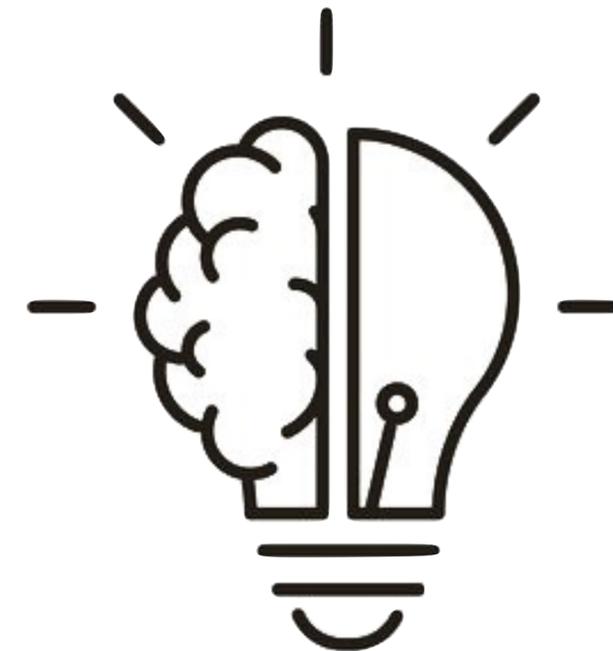
# How can AI help?

- AI's impact in research ranges from **search** to **discovery**



## Search

Accessing knowledge in data



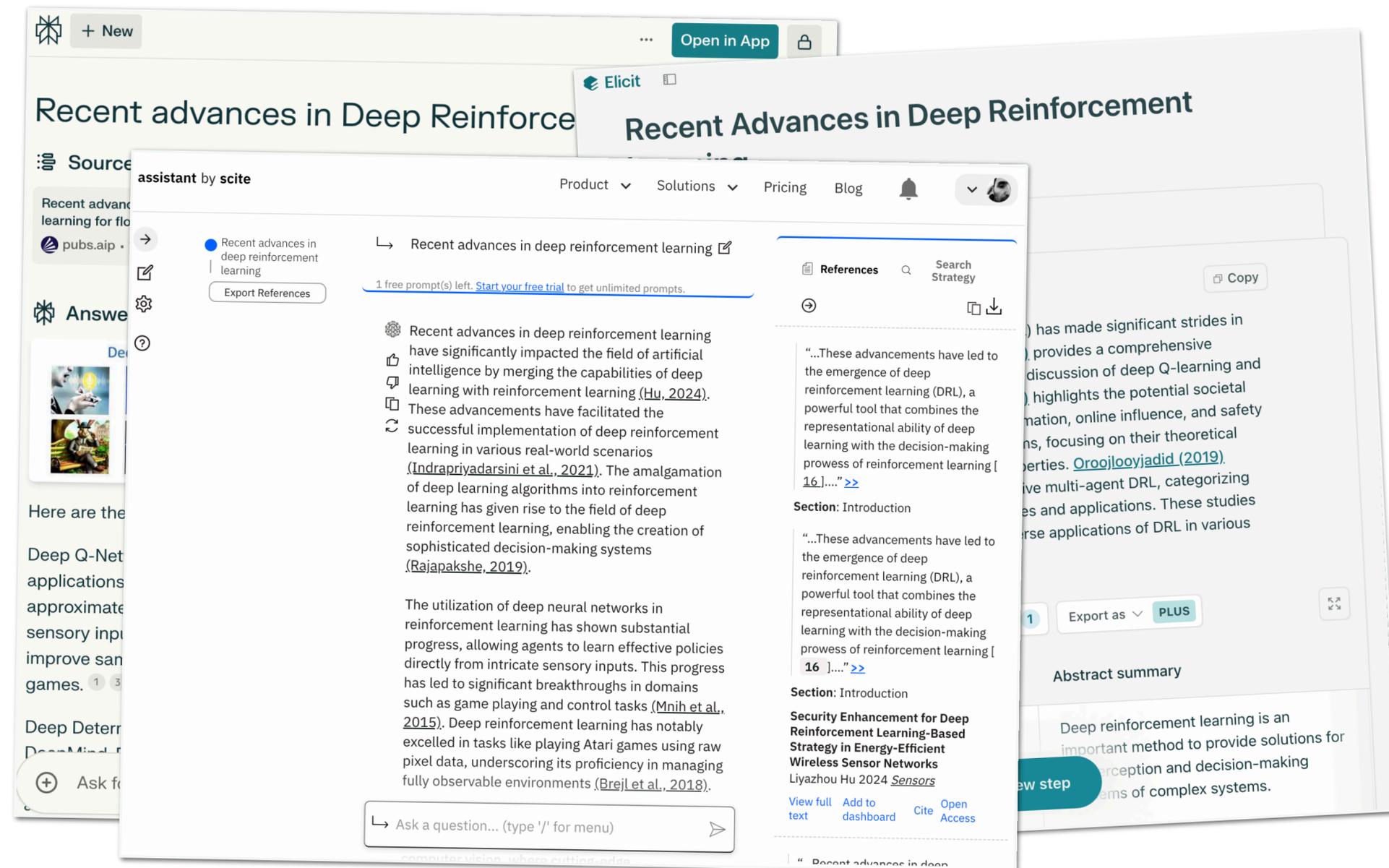
## Discovery

Identify new patterns in an open-ended manner

# Tools

Literature review (summarization, reference search)

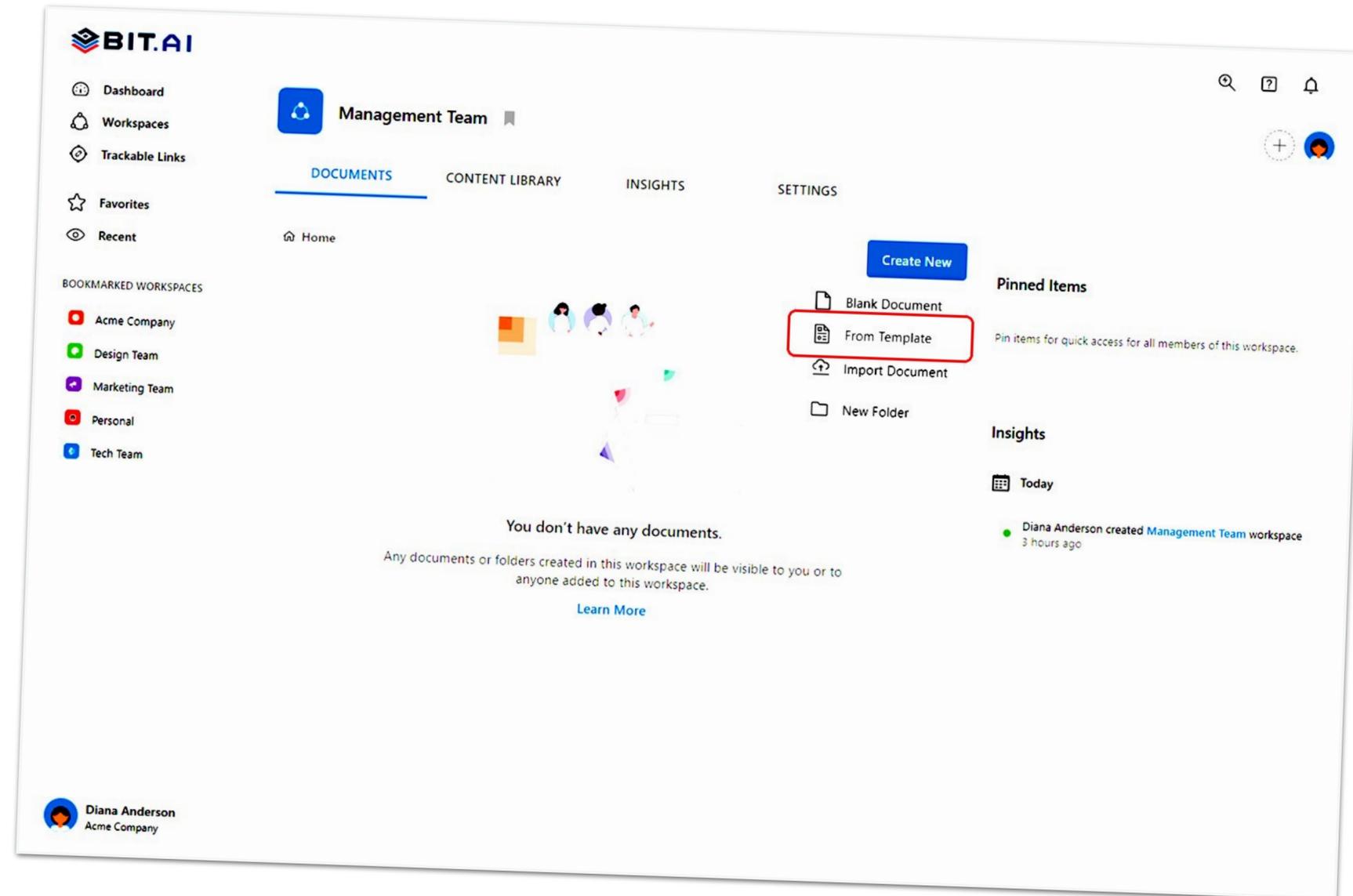
- Scite ([scite.ai](https://scite.ai))
- Elicit ([elicit.com](https://elicit.com))
- Perplexity ([perplexity.ai](https://perplexity.ai))



# Tools

Support to document production and collaborative writing

- Bit AI ([bit.ai](https://bit.ai))



# Caveats

- Although these tools can help, texts produced by AI tend to be verbose and exhibit complex language
  - This can impact the clarity of the message you are trying to convey
- Using these tools, for example, to write paper reviews may not be well accepted by authors
  - Authors expect to have their papers reviewed by peers and receive constructive criticisms

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