



AI for science, science for AI



UAR 2036 - Centre AISSAI
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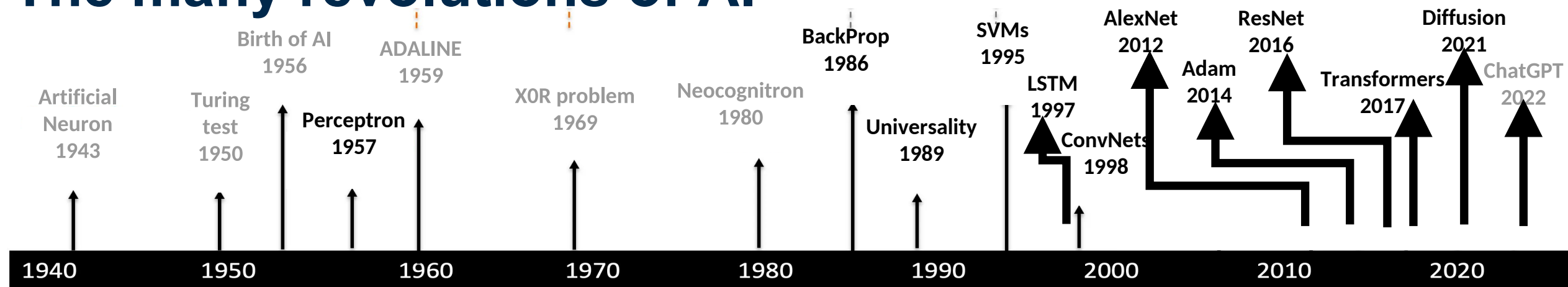
→ 26/11/2025



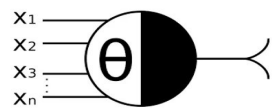
AI and Science

- Scientists strive to **understand** how **nature** and **society** work.
- They formulate **hypotheses**, design **experiments** and collect **data**, analyze them to better understand **natural, physical and social phenomena**.
- Data **collection** and **analysis** are central to the scientific method: scientists have long used statistical techniques to **extract information from data, test and (in)validate hypotheses**, etc.
- **Statistical methods** are ubiquitous in **scientific methodology** and numerous examples can be seen throughout history, from astronomy to genomics.

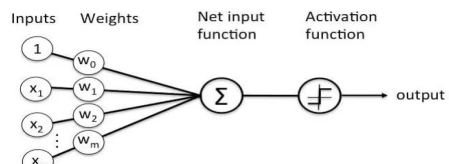
The many revolutions of AI



McCulloch-Pitts

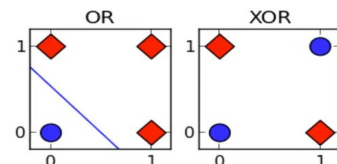


Rosenblatt

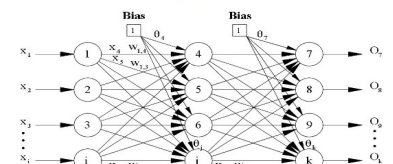


Widrow-Hoff

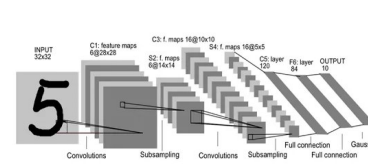
Minsky-Papert



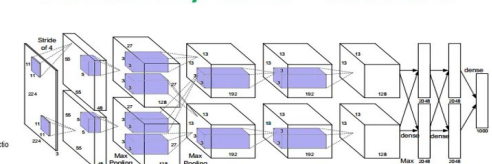
Rumelhart, Hinton et al.



LeCun



Hinton-Ruslan Krizhevsky et al.



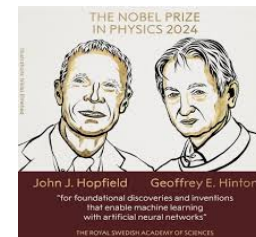
Vaswani

AI provides new tools and is becoming a **knowledge discovery paradigm** impacting the way research is produced across disciplines.

AI is also **nurtured** by other **disciplines**: physics, mathematics, neuroscience, etc.

This paradigm change was spectacularly illustrated by the 2024 edition of the **Nobel Prizes**: Nobel Prize for Physics (neural networks) and The Nobel Prize for Chemistry (AlphaFold).

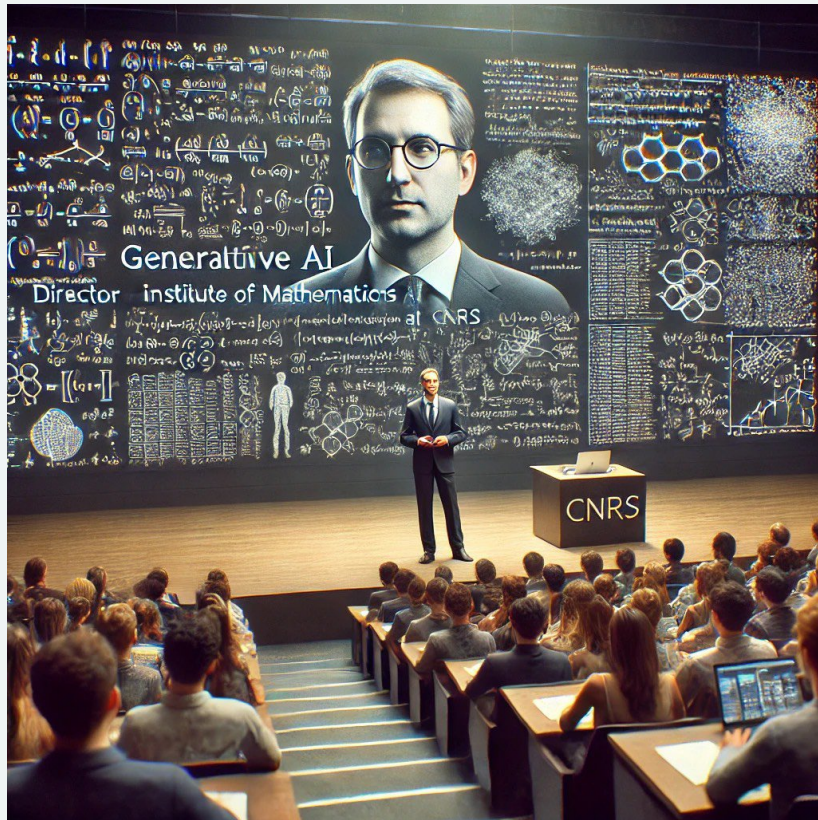
These two prizes are a perfect illustration of the **cross-fertilization** between **AI and science**.



Strategic view: from AI to Generative AI in Sciences

Images

Le directeur de CNRS Mathématiques en train de présenter l'IA générative devant un large auditoire.



DALL-E 2

stability.ai



Text

Raconte de façon rigolotte l'histoire du directeur de CNRS Sciences Informatiques qui présente l'IA générative devant un large auditoire.



Le professeur Claire Leclair, célèbre directrice de CNRS Sciences Informatiques, monte sur scène avec l'enthousiasme d'un enfant qui vient de découvrir que son yaourt préféré a un nouveau goût. Devant elle, un large auditoire aux regards curieux. "Aujourd'hui, mes amis," commence-t-elle avec un clin d'œil complice, "je vais vous prouver que les mathématiques et l'informatique peuvent être aussi sexy qu'un chaton jouant avec une pelote de laine... et je parle bien sûr de l'IA générative!". D'un geste dramatique, elle appuie sur sa télécommande, et l'écran derrière elle se remplit d'équations complexes et de codes qui dansent comme des notes de musique sur un karaoké.



Strategic view: from AI to Generative AI in Sciences

Terminology : « Large Language Model » (LLM)

« foundation models »

Large neural networks

Trained to generate data
... or solve problems

Can be fine-tuned at low cost

Prouve que le produit scalaire matriciel $\langle S, T \rangle$ peut s'écrire $\text{tr}(ST^t)$.



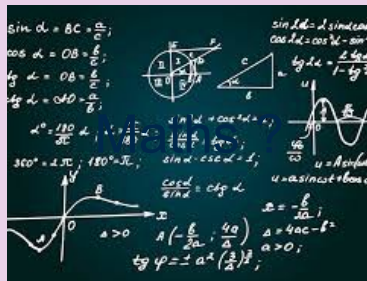
LE CHAT
MISTRAL

Pour prouver que le produit scalaire matriciel $\langle S, T \rangle$ peut s'écrire sous la forme $\text{tr}(ST^t)$, considérons les définitions suivantes : le produit scalaire entre deux matrices S et T de taille $n \times n$ est donné par $\langle S, T \rangle = \sum_{i=1}^n \sum_{j=1}^n s_{ij} t_{ij}$. La trace du produit ST^t est définie comme $\text{tr}(ST^t) = \sum_{i=1}^n (ST^t)_{ii}$. En développant l'élément diagonal, nous avons $(ST^t)_{ii} = \sum_{j=1}^n s_{ij} t_{ij}$, ce qui donne

$$\text{tr}(ST^t) = \sum_{i=1}^n \sum_{j=1}^n s_{ij} t_{ij} = \langle S, T \rangle.$$

Ainsi, $\langle S, T \rangle = \text{tr}(ST^t)$.

How to extend these methods beyond text and images ?



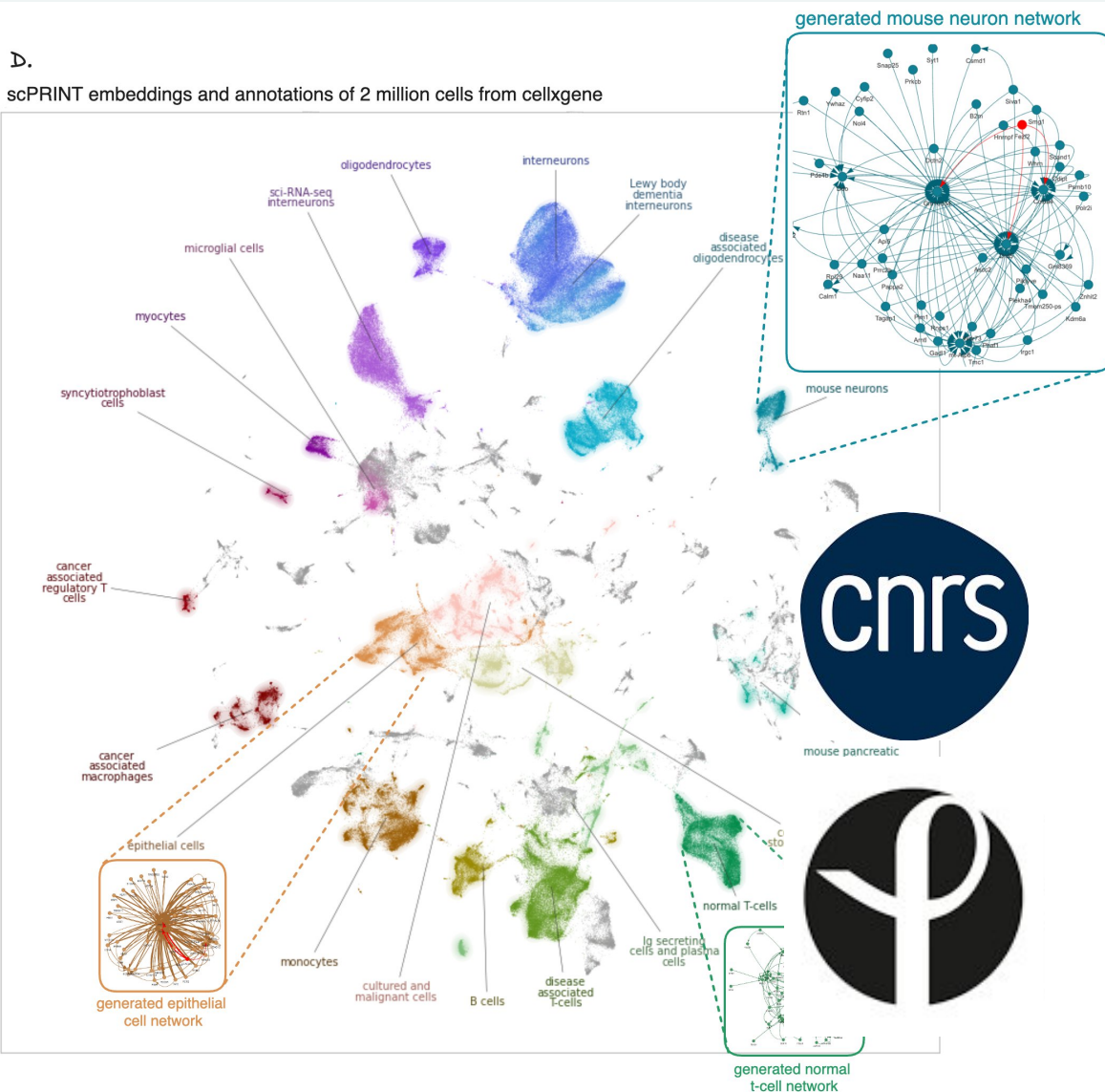
...

A whole program of theoretical, practical and societal questions

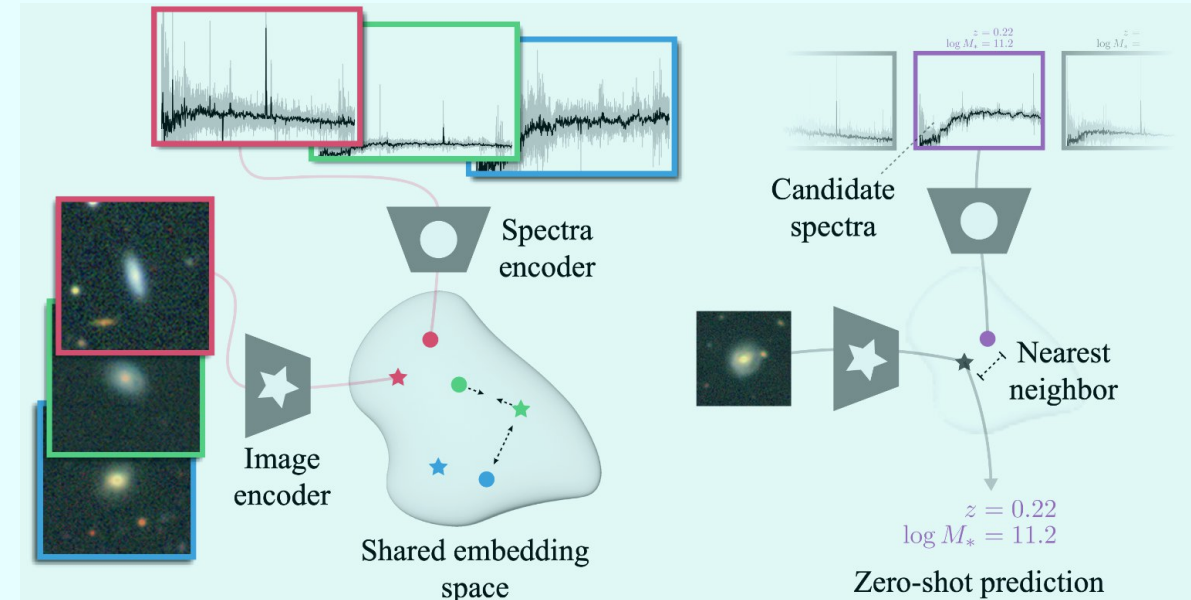
AI in genomics and physics

scPRINT: Large Cell Model for scRNAseq data

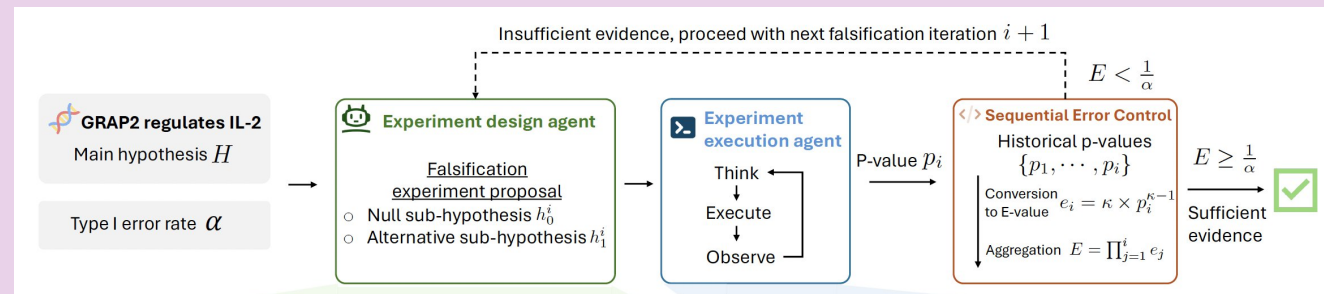
D.
scPRINT embeddings and annotations of 2 million cells from cellxgene



AstroCLIP: A Cross-Modal Foundation Model for Galaxies



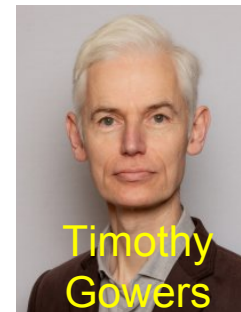
Automated Hypothesis Validation with LLM Agents Popper's principle of falsification



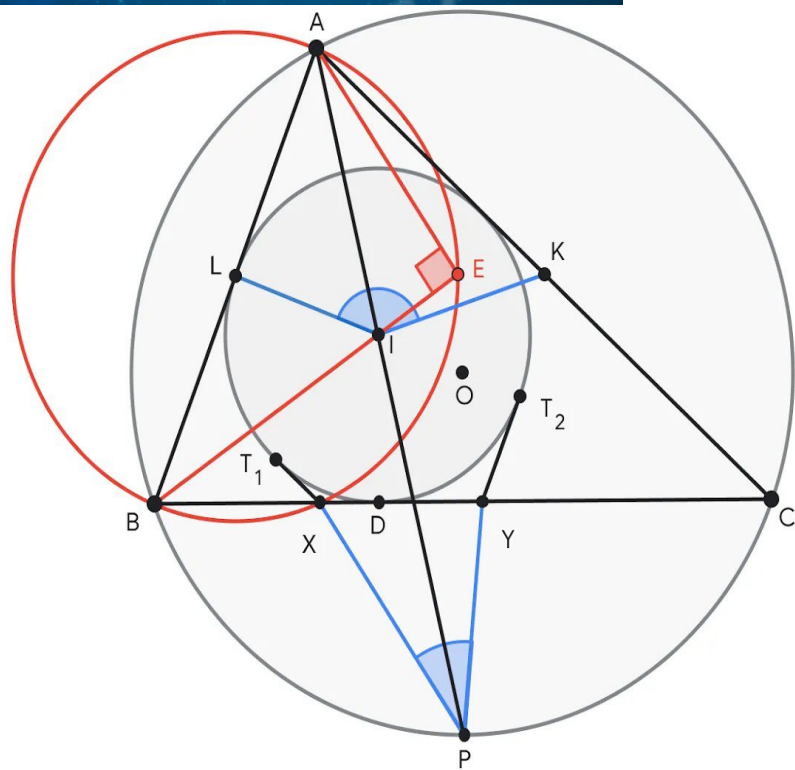
Example of mathematics and CS



« LLM-guided evolutionary search can autonomously discover mathematical constructions that complement human intuition, at times matching or even improving the best known results, highlighting the potential for significant new ways of interaction between mathematicians and AI systems. »



« The fact that the program can come up with a non-obvious construction like this is very impressive, and well beyond what I thought was state of the art. »



Show that $\angle KIL + \angle XPY = 180^\circ$

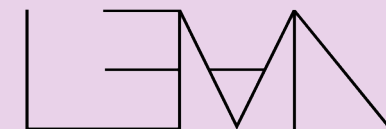
Reasoning models: Chain of thoughts, Test time scaling, RL.

AlphaEvolve: LLM coding agent for algorithmic solutions to scientific problems.

AlphaProof: formal reasoning.

DeepThink: informal reasoning.

Interaction with formal proof languages



<https://www.renaissancephilanthropy.org/ai-for-math-fund-projects>

AI@CNRS

- **AI** methods face important challenges when modeling **increasingly complex and multiscale systems**, exploiting the **massive increase** in flow, volume and diversity of **multi-source/physics data** from large instruments, observation systems, experimental platforms, etc.
- In science, **data** can be (very) **expensive** to generate and collect.
- AI methods lead to **new research practices** whose level of maturity and organization varies greatly from one discipline to another.
- Within the CNRS, AI methods are now being **deployed very rapidly** in the context of major research infrastructures and experimental platforms: e.g., biology, high-energy physics, earth and universe sciences, climate modeling, ecology, material sciences, etc.

AI@CNRS

- For CNRS, it is key to address AI from an **holistic standpoint**.
- Scientific organizations like the CNRS have responsibility to **help policy makers and public opinion** understand the implications, benefits and possible risks of AI.
- Within the National strategy in AI (SNIA, 2018), CNRS has been actively involved in several AI programs:

➤ 9 AI clusters.

➤ Choose France – CNRS AI Rising talents.



➤ CNRS operates the **Jean Zay** national supercomputer for AI and **engineers network (PNRIA1 and PNRIA2)**.

➤ Co-coordination of the **PEPR AI** oriented towards trustworthy, embedded and decentralized AI.

➤ Creation of **AISSAI** center.

• International Research Labs with activities in AI

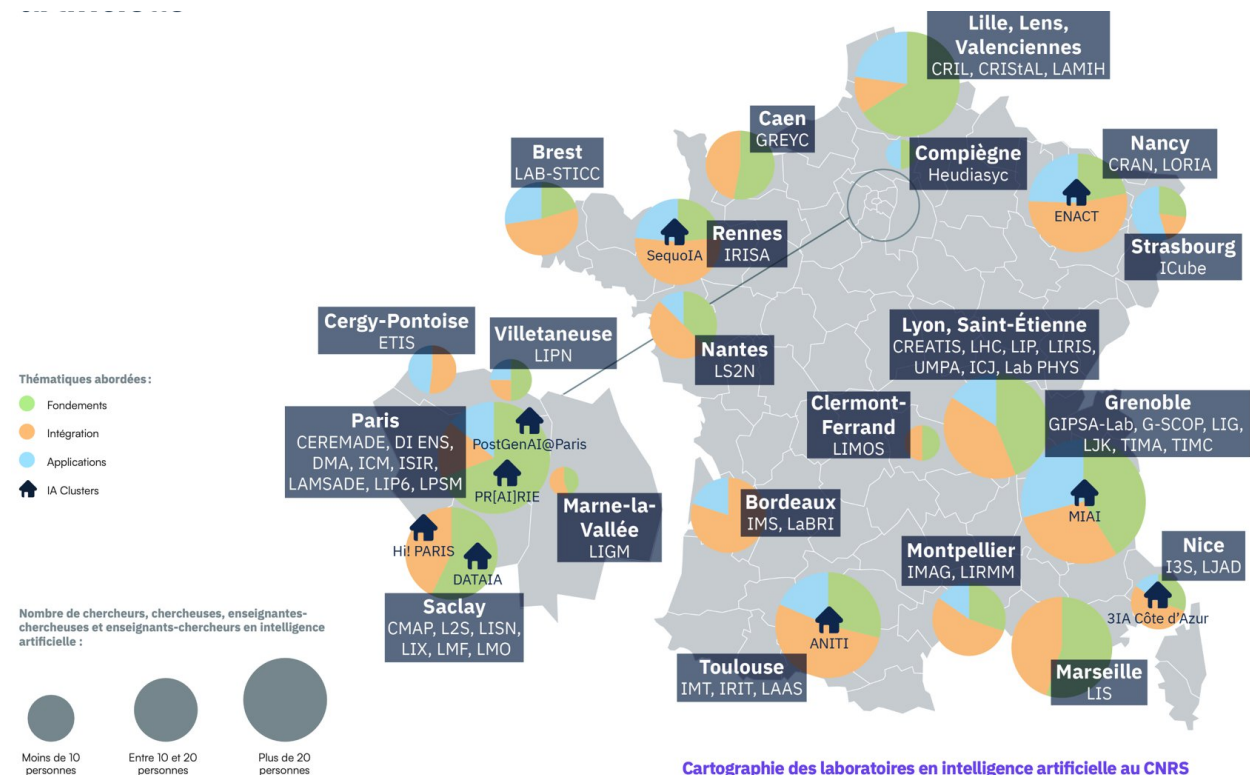
Singapore – IPAL + DESCARTES CREATE Program (2021-)

Japan – JFLI (Tokyo)

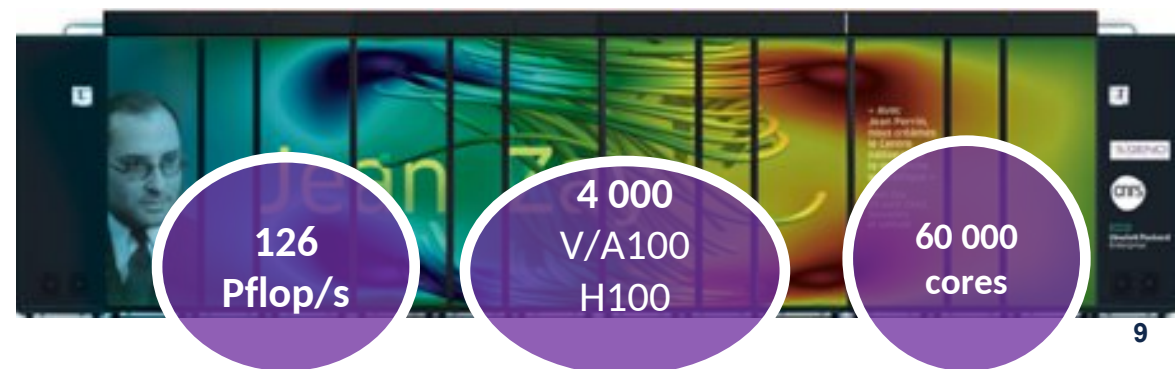
Australia – CROSSING (Adelaide), with Naval Group (2021-)

Canada – ILLS (Montreal, 2022-)

French academic research in AI



Cartographie des laboratoires en intelligence artificielle au CNRS



AISSAI

AISSAI is one of the most **emblematic** actions of the **CNRS** in the field of **AI**
CNRS spans the **whole spectrum of sciences**

- Early 2020 : AI as a social challenge WG of multiannual contract 2019-2023



- End 2021 : the WG proposed to create a multidisciplinary center dedicated to AI for Science and Science for AI



- Jan. 1st 2024 : UAR 2036 CNRS Informatics and Mathematics.
- A cross-disciplinary center to all CNRS departments.
- No premises of its own. Staff located at CNRS Informatics.

Goals of AISSAI

IHP of AI

Support **science for AI** research and the integration of **AI into research practices**

Foster dialogue between scientific disciplines in interaction with AI

Address **domain-specific strategic questions**

Structure the AI strategy of CNRS across **all institutes**

Establish **new modes of collaboration** beyond the mere assimilation of AI

Accelerate scientific discovery in all CNRS spectrum

Build ties with other similar centers abroad.

Governance

Conseil Scientifique International

Tanya Berger Wolf (Ohio State Univ)

Stephen Cave (Cambridge)

Claudia Draxl (Humboldt Univ Berlin)

Antoine Georges (Collège de France)

Alfred Hero (Univ Michigan & NSF)

George Karniadakis (Brown Univ)

Emma Lundberg (Stanford)

Brice Ménard (Johns Hopkins)

Jesse Thaler (MIT)

Rebecca Willett (Univ Chicago)

Directeur

Jalal Fadili *

(Pr, ENSICAEN)

Comité de Pilotage

(membres représentant les dix instituts du CNRS, la MITI et la DGDS)

Massih-Reza Amini

Pr, Univ Grenoble Alpes
CNRS Sciences informatiques

Marc Baaden

DR, CNRS
CNRS Chimie

Matteo Cacciari

Pr, Univ Paris Cité
CNRS Physique

Julien Donini

Pr, Univ Clermont Auvergne
CNRS Nucléaire & Particules

Alexandre Gefen

DR, CNRS
CNRS Sciences humaines & sociales

Fabien Godeferd

DR, CNRS
CNRS Ingénierie

Martina Knoop

DR, CNRS
Mission pour les Initiatives
Transverses et Interdisciplinaires
(MITI)

Arnaud Lalo

IR, CNRS
Direction Générale Déléguée à la
Science (DGDS)

Vincent Miele

IR, CNRS
CNRS Écologie & Environnement

Perrine Paul-Gilloteaux

IR, CNRS
CNRS Biologie

Gabriel Peyré

DR, CNRS
CNRS Mathématiques

Jean-Pierre Vilotte

Pr, IPGP
CNRS Terre & Univers

Administration

(hébergée par CNRS Sciences
informatiques)

Secrétaire Général

Vincent Folliard *

(IR CDD, CNRS)

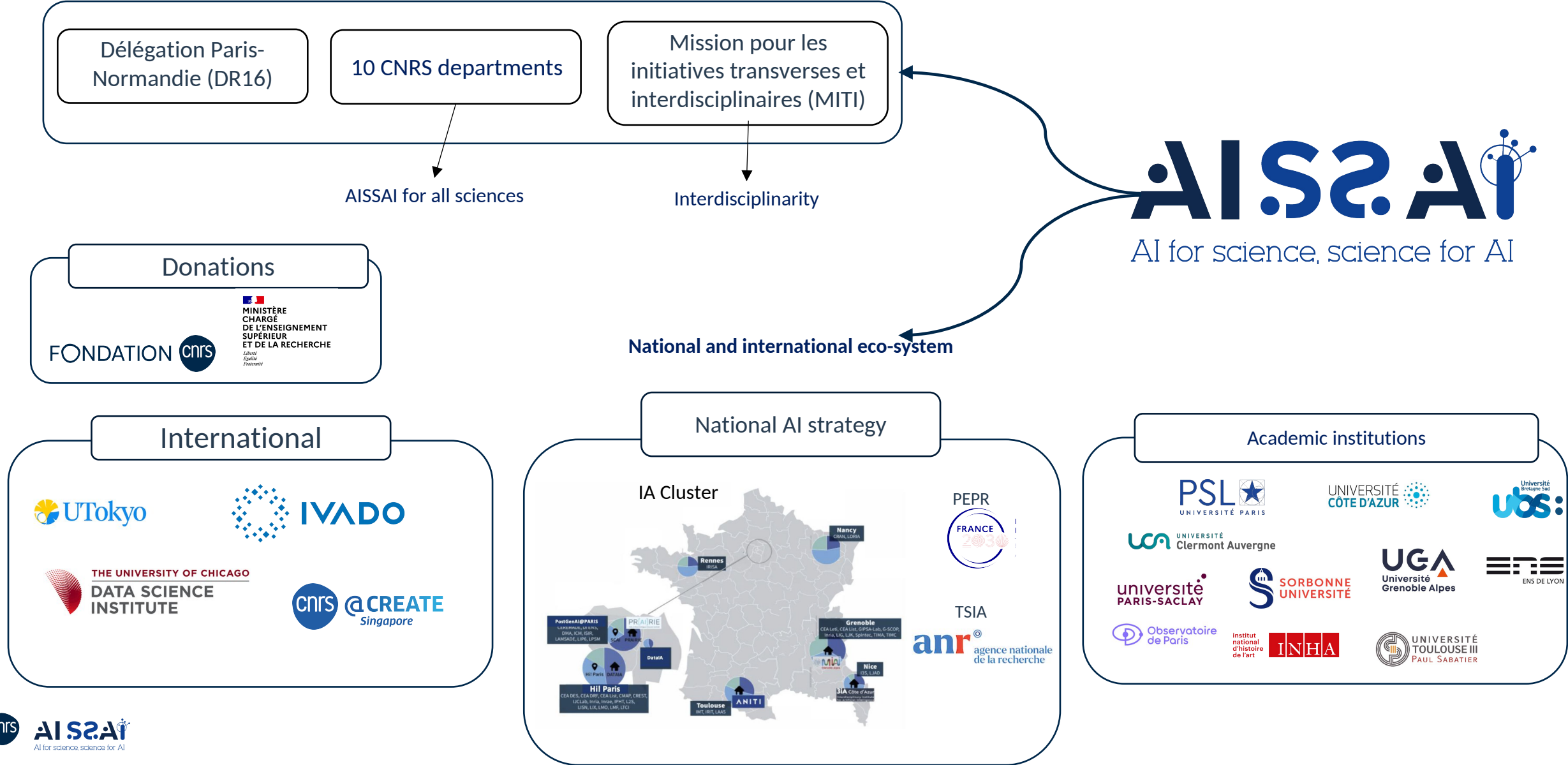
Assistante en gestion financière

Célina Nsikatia *

(AI CDD, CNRS,
Poste partagé à 50% avec CNRS
Sciences informatiques)

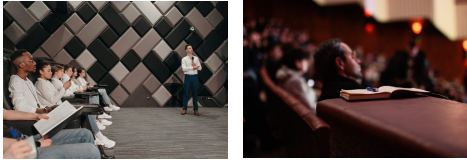
* Personnel appartenant à l'unité AISSAI center

AISSAI environment



Scientific actions

Thematic semesters on AI&Sciences (2/y)



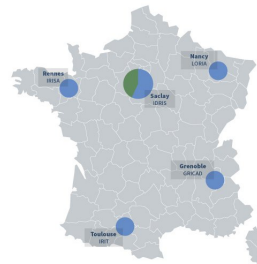
Training AI&Science



Workshops, seminars, hackathons



AI engineers on multidisciplinary projects

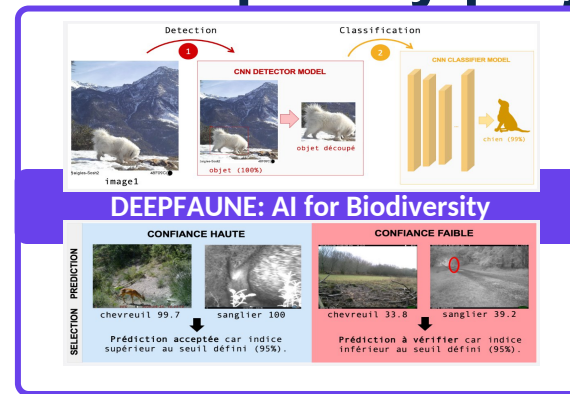


PhD and postdoc programs



1-2 year chair program

Host multidisciplinary teams



International cooperation

- Build strong ties with **similar centers abroad** ➔ **international network**.
- We have been approached by several centers abroad to forge links and collaborations: IVADO (Québec), U. of Chicago, IRC U. Tokyo, Singapore.
- **IVADO:**
 - A roadmap has been drawn up and is currently under implementation.
 - **Working groups** on specific subjects: **neuroscience, materials and molecule discovery, environmental sciences, AI and the human in the loop**.
- **U. Tokyo:**
 - Working group with U. Tokyo on IA and Science (extreme events).
- **U. Chicago:** summer school 30 June-4 July 2025. Will become a regular event.
- **Google:** 1M€ donation to Fondation du CNRS. Post-doc calls.

Post-docs call: CNRS Foundation, Google donation

- Call for 6 post-doctoral fellowships of 18 months.
- 1 project: at least 2 institutes, 2 units, AI and Sciences.
- 55 applications received (top-down campaign targeted by institutes).
- Very high quality of applications.
- 25 shortlisted.
- International expertise.
- Dec. 6, 2024: 6 on main list, 3 on complementary list.
- Eventually 8 funded thanks to an additional funding: physics, chemistry, biodiversity, climate, geophysics, genomics, biology, particle physics, mathematics, quantum informatics.
- Additional funding for next year edition.
- Collaborations between Google researchers and our PIs on some projects.
- Kick off meeting Nov. 14 with a fireside on AI and Science.

AISSAI in Europe

G6

CNRS (FR)
Helmholtz Association (GER)
CSIC (ESP)
CNR (IT)
Max Planck (GER)
Leibniz Association (GER)

EuroHPC

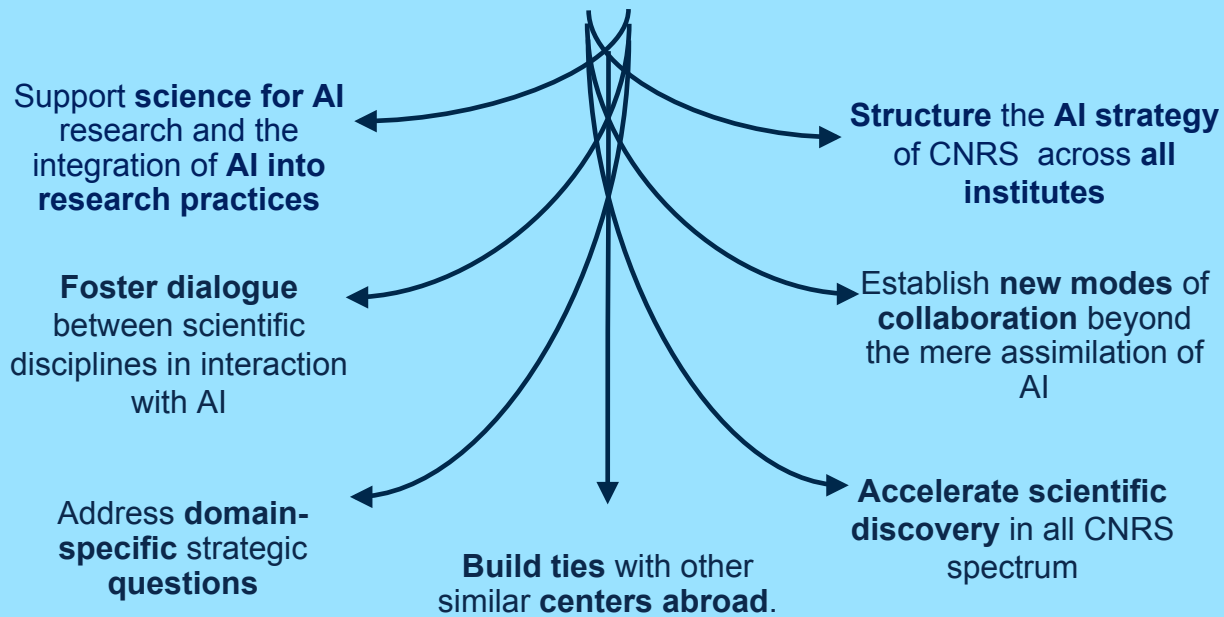
Minerva project
Italie, France, Espagne,
Allemagne, Finlande

European commission

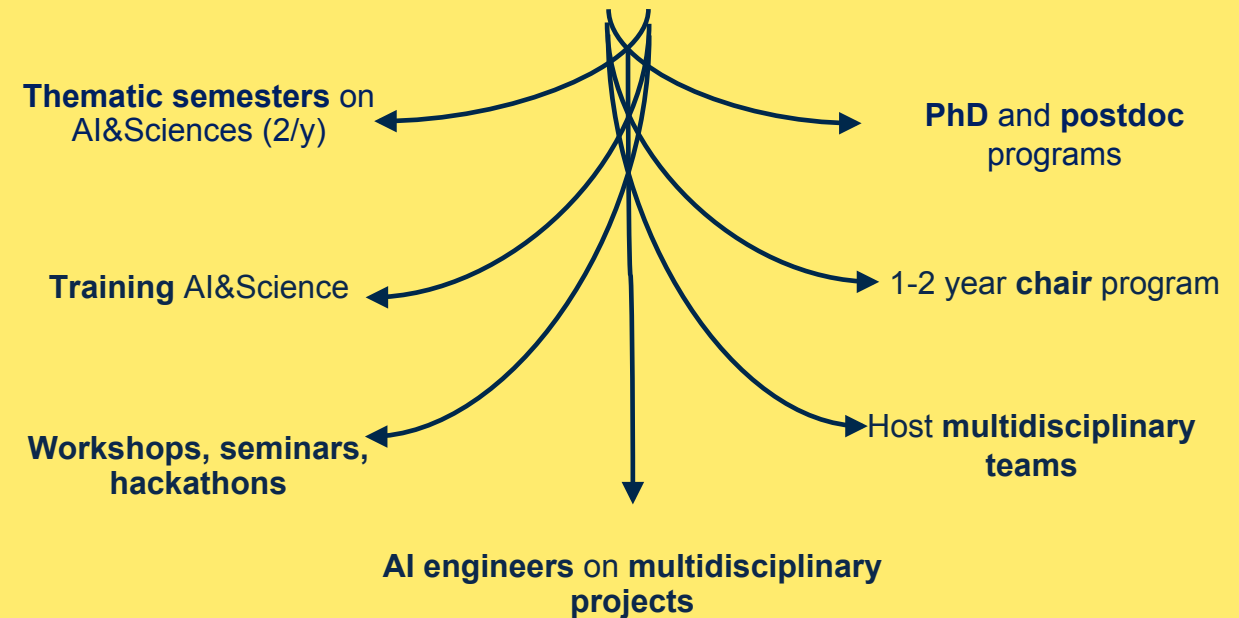
AI Continent Action Plan
RAISE
ERA Action 'AI in Science'
Position papers

ELLIS, CLAIRE, EMBL,
CERN, etc.

Ambition of AISSAI



Scientific actions



International and European cooperation

Build strong ties with similar centers abroad → international network.



- Ongoing 5-year cooperation program with IVADO.
- Several events with U. Chicago.
- Discussions with CREATE for an AISSAI center in Singapore.
- Funding and cooperation with Google.

CNRS driving force in AI and Science foresight and strategy at national and European level



<https://aissai.cnrs.fr/>



CNRS
AISSAI CENTER

