Research, Science an Computational Sciences

Guillaume Beslon

5IF – Tronc Commun Scientifique – TCS2

Year 2022/2023

Foreword:

These slides are available at:

https://moodle.insa-lyon.fr/course/view.php?id=3985

Introduction: Who am I?

- Guillaume Beslon (guillaume.beslon@insa-lyon.fr)
- Professor at INSA-Lyon
  - Computer architecture (3IF-AC)
  - Introduction to data-management (3BS-COINFO1)
  - Computational sciences (5IF-TCS2)
  - Projet Scientifique Artistique et Technique (5IF-P-SAT)
- Head of the “Beagle” research team (INRIA/LIRIS)
  - Computational Biology and Artificial Evolution
  - Artificial Life and Computational Neurosciences

  → Personal research topics: Computational Evolution
- Coordinator of the artistic option ``light and sound'' (ake ``teck'') at the humanities department of INSA-Lyon
- Warning: My office is NOT in the Ada Lovelace building... You'll find me at the Inria center (CEI-2 building) → send a mail (or two :-/)

Introduction

- ``Tronc Commun Scientifique''
  - Introduction to research
  - Four lectures
    1. ~~TCS0 : Le contexte scientifique contemporain (J.-F. Boulicaut)~~
    2. TCS1 : Theoretical Computer Science (C. Solnon)
    3. TCS2 : Computational Sciences (G. Beslon)
    4. P-SAT
- The aim of computational sciences et to do science **with** computers (not to do science **of** computers) …
  - All scientific domains are involved
  - In this lecture, we will specifically focus on ``complex systems''
- Part of this lecture will also contain some elements of former TCS0 by J.-F. Boulicaut ...

Introduction

- Schedule (will evolve :-/)
  - Wednesday October 19th, 8h-10h (now ;)
  - Wednesday October 26th, 8h-10h
  - Wednesday November 9th, 10h-12h
  - Wednesday November 23th, 10h-12h
  - Wednesday November 30th, 10h-12h
  - Wednesday December 7th, 10h-12h
  - Wednesday December 14th, 8h-12h and 14h-18h → WILL BE MOVED
  - Wednesday January 18, 10h-12h
- The course is constructed as a series of lectures and debates...
  - It involves discussion!
- Evaluation
  - Shared evoluation with TCS-1 (Wednesday February 1st, 10h-12h)

Research, Science an Computational Sciences

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Foreword

« Un enseignement de la science qui n'apprend pas à penser n'est pas un enseignement de la science, il est un enseignement de la soumission. »

E. Schatzman,
Science et société, 1971

Let’s discuss a little...

Science

Research

Scientific research

Epistemology

Innovation

Progress

Scientific method

Computational science

Discutons un peu ...

Science

Recherche

Recherche scientifique

Epistémologie

Innovation

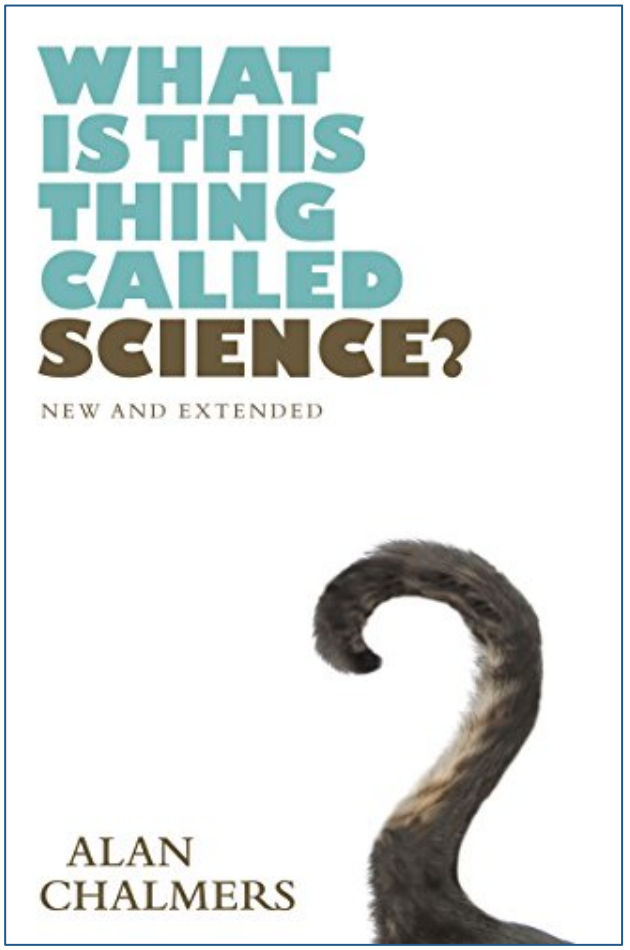
Progrès

Méthode scientifique

Sciences computationnelles

What is science?

- In fact, we don't really know what!
  - This is one of the roles of epistemology
  - Alan F. Chalmers identifies at least 5 currents of thought defining science!
    - Inductivism
    - Falsificationism
    - Rationalism
    - Objectivism
    - Non-figurative realism
- BUT, it’s an important thing!
  - A.F. Chalmers : « Science is highly esteemed. Apparently it is a widely held belief that there is something special about science and its methods. The naming of some claim or line of reasoning or piece of research "scientific" is done in a way that is intended to imply some kind of merit or special kind of reliability »



→ Why is this so? What gives science this “esteem”? This “merit”, this “special kind of reliability”?

Let’s discuss a little...

Science

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Scientific research

Epistemology

Innovation

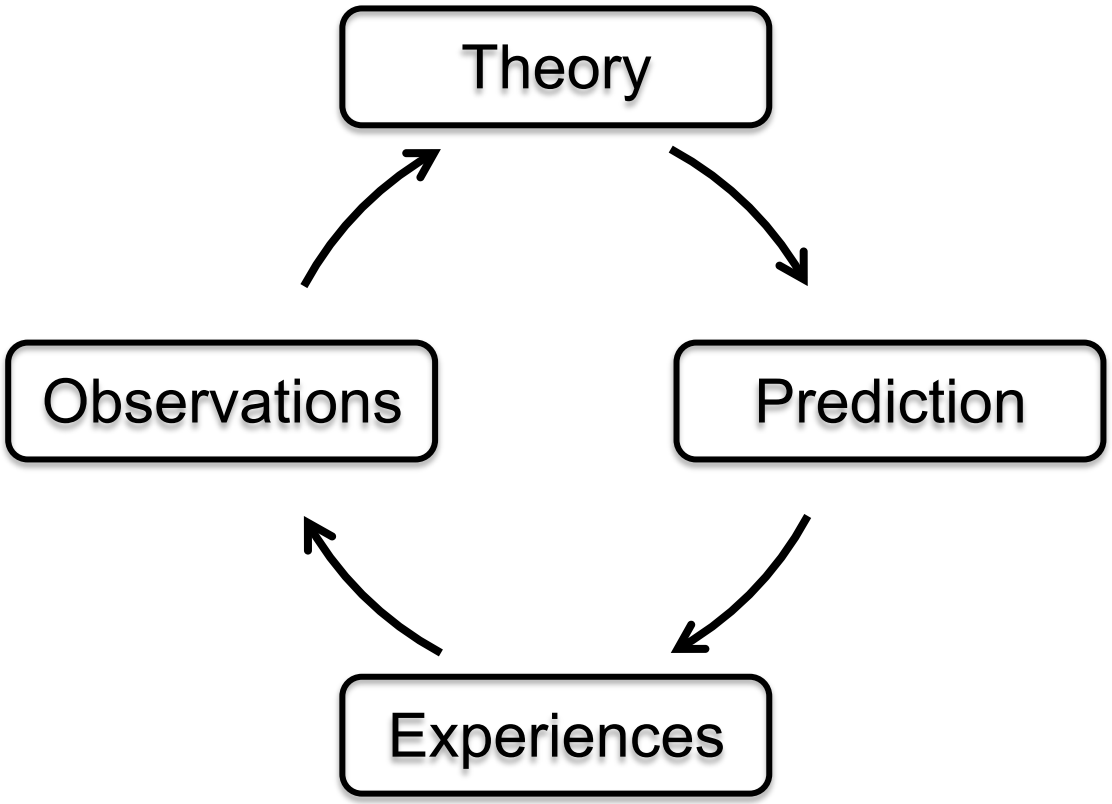
Progress

Scientific method

Computational science

The scientific method: How is science done?

- The two legs / pillars of science:
  - Logic and observation (or theory and experiment)



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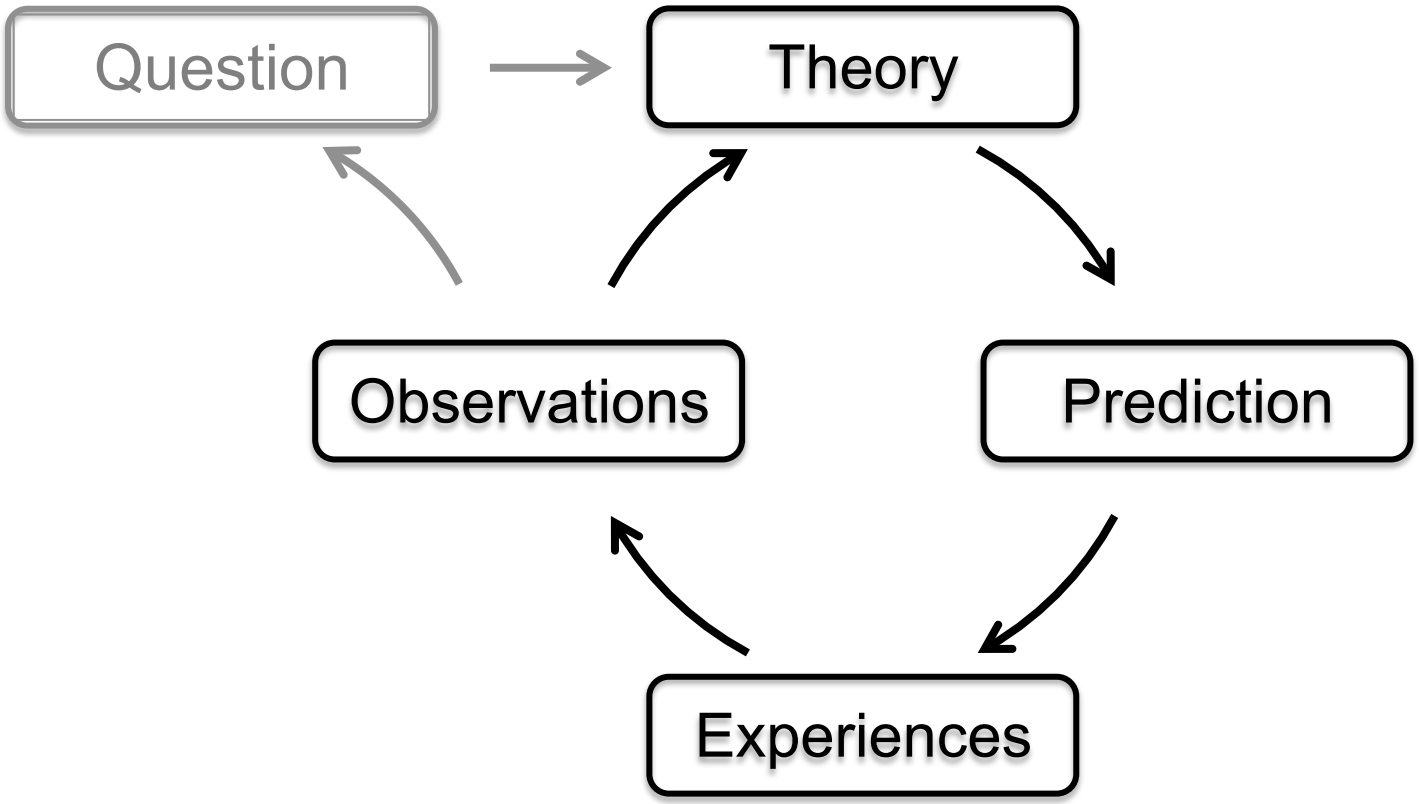
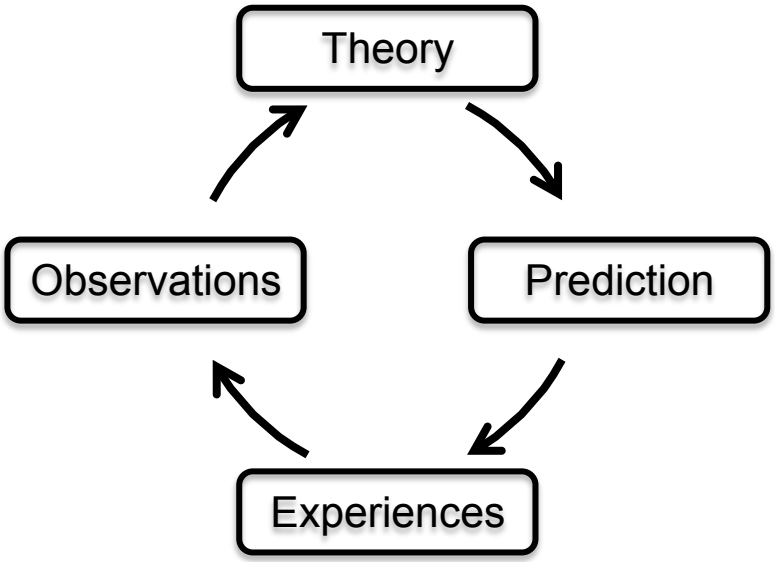


La méthode scientifique : comment fait-on la science ?

- The two legs / pillars of science:
  - Logic and observation (or theory and experiment)
  - Starting from a sceptical view of the world (“Questioning”)
  - Rational approach to ensure confidence in scientific results, thus in theories and their predictions!
  - The 'value' of science is based on confidence in scientific predictions which are :
    - Independent of opinion
    - Falsifiable
    - Universal



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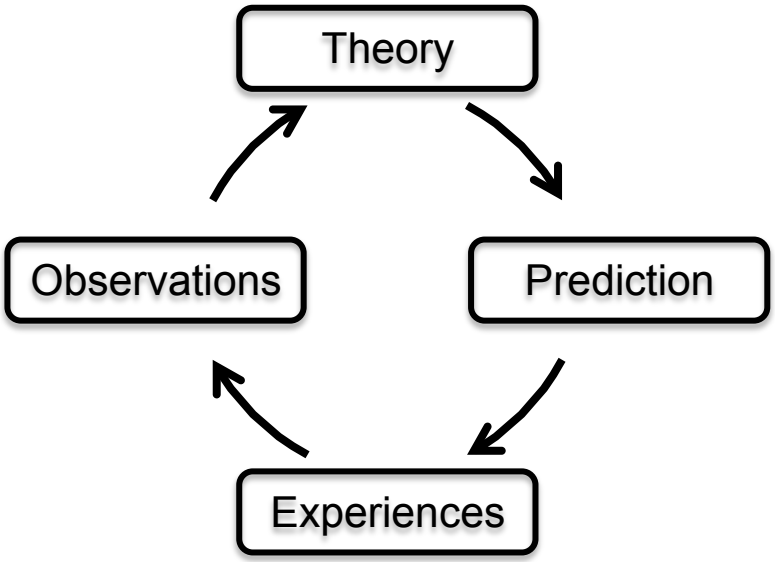
⇩

The results of science are systematically (!) subjected to peer review...



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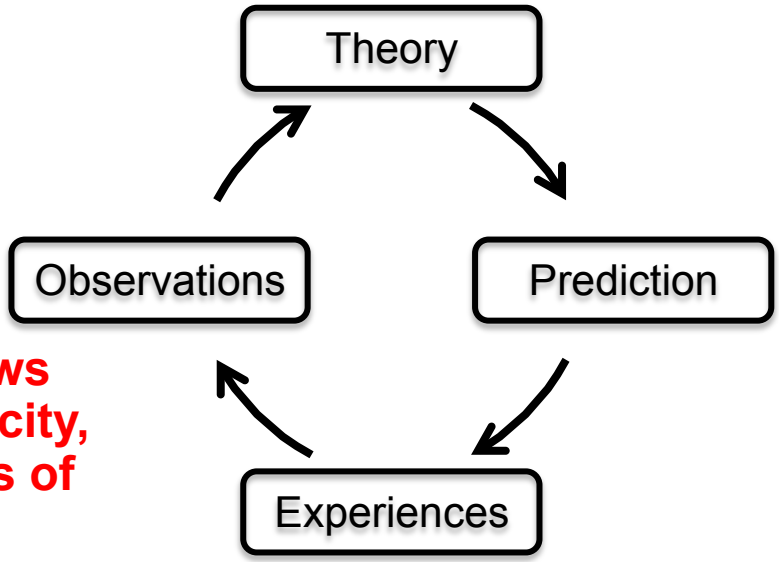

Confidence in the results of science allows it to be used for politics...(governing the city, making collective decisions...) regardless of beliefs

Hmm not so simple...

Science

Research

Scientific research

Epistemology

Innovation

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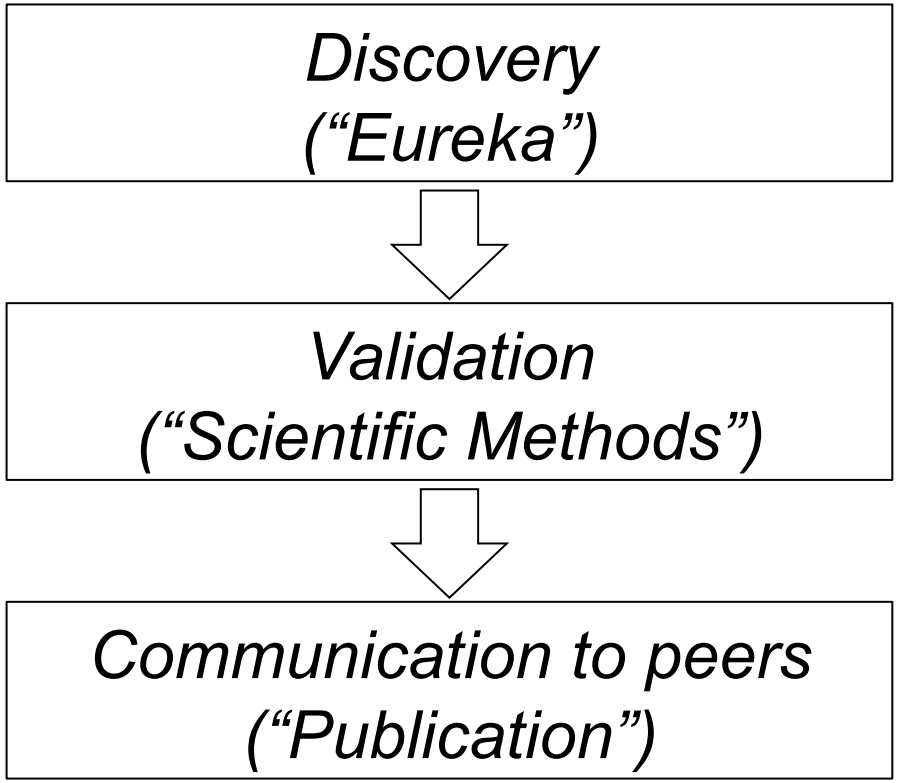
But the scientific method is only part of the scientific process!!

- Research goes through three very distinct phases
- The scientific method is only phase 2!



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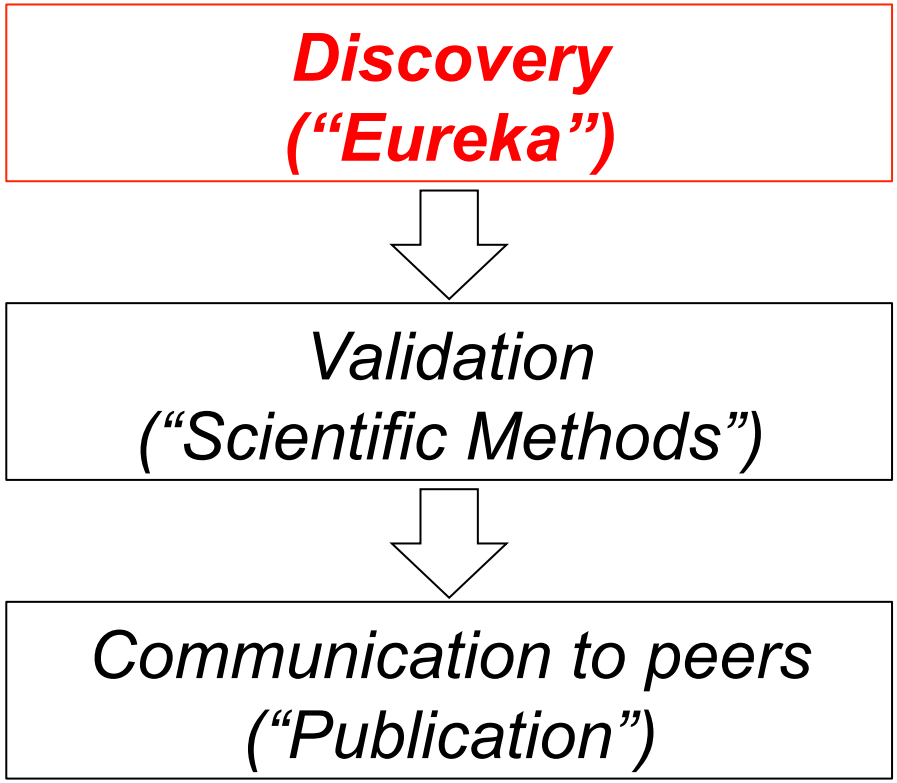

- What fuels discovery?
- In science, chance favors only the prepared mind (according to Louis Pasteur)
- Questioning and discovery are intimately linked (even if nobody says so!). Questions are often reformulated after the results are obtained!

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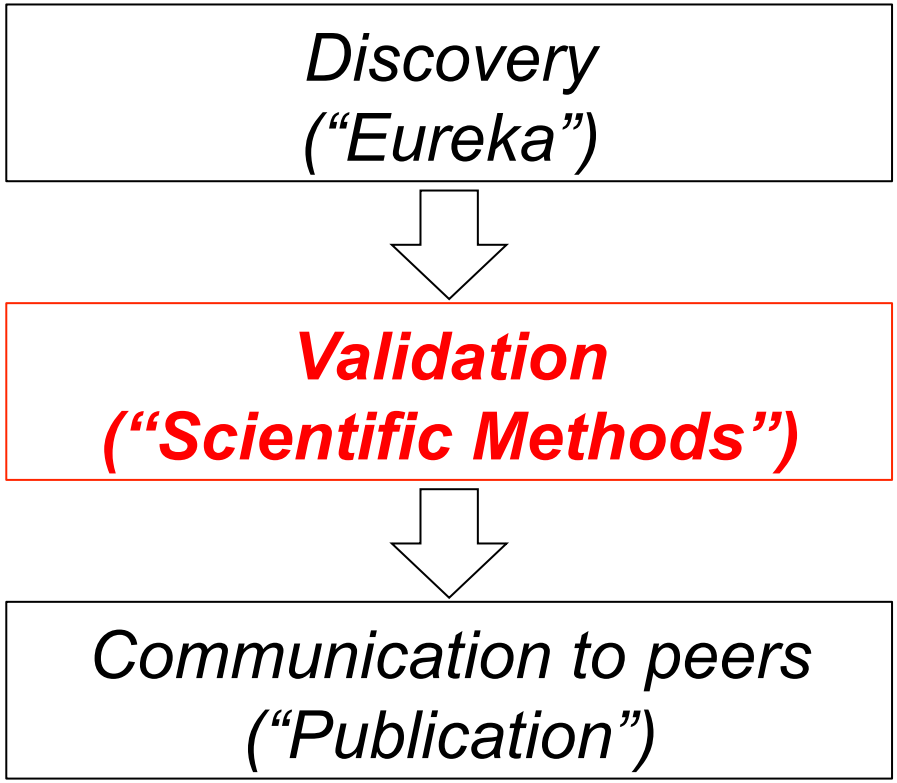

- There is not ONE scientific method but MANY scientific methods
- It is the field of research that determines what is scientifically admissible or not (i.e. the method)
- So, is it really that rigorous?

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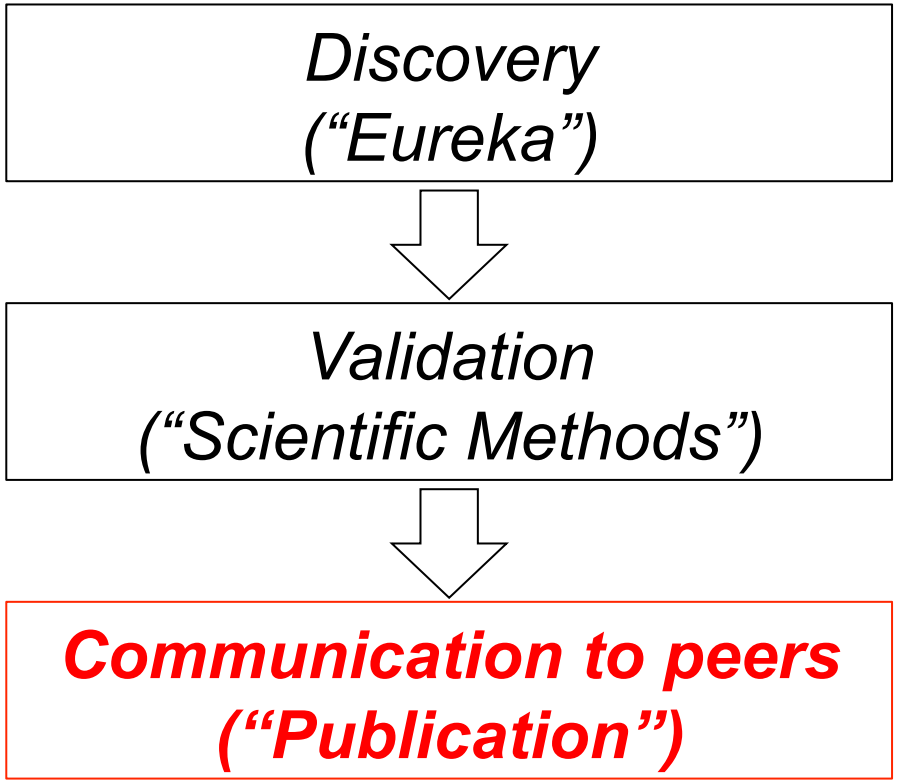
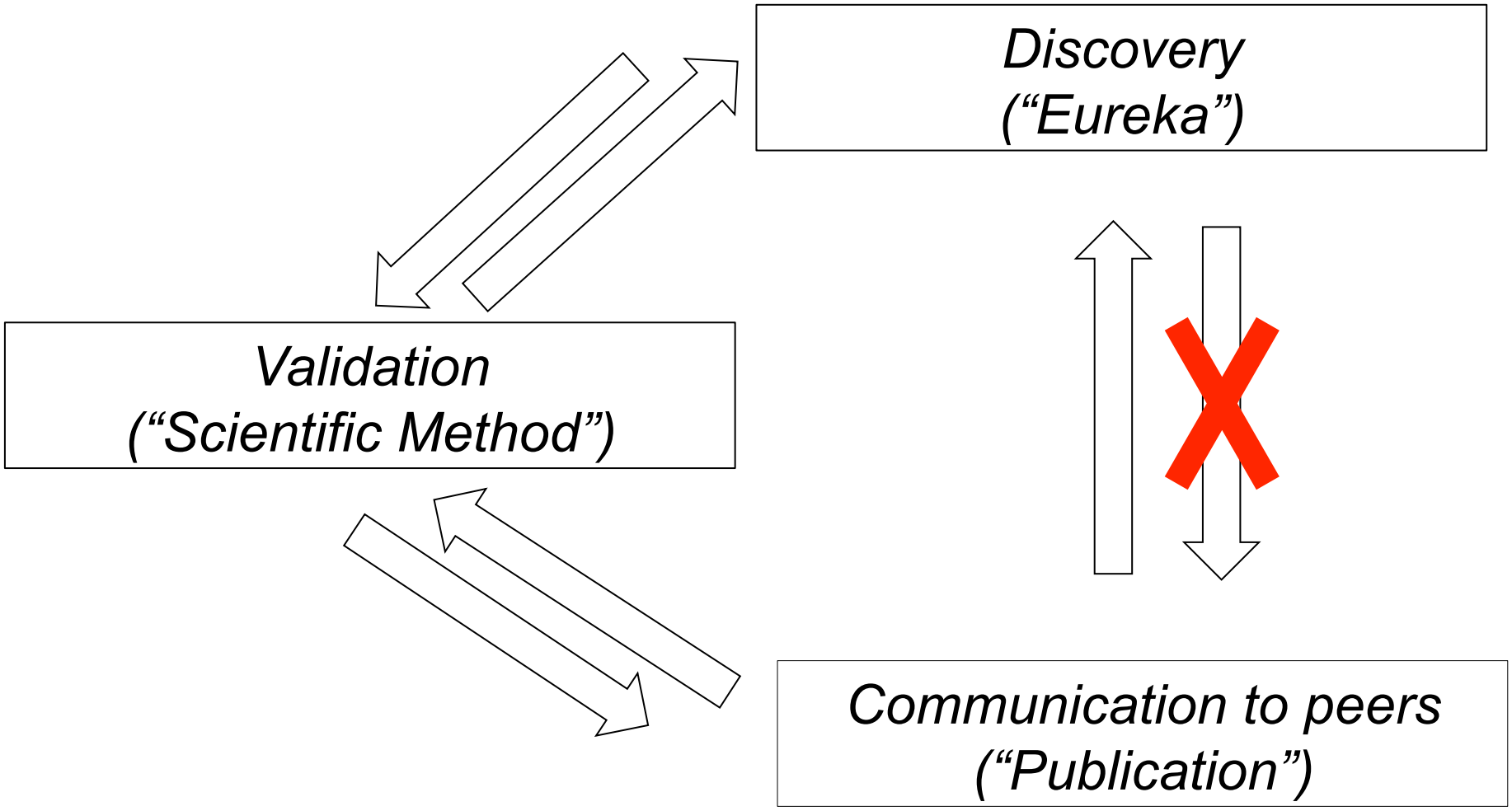


- Publications (scientific journals)
- Communications (scientific conferences)
- Oral presentation
- Poster
- Grey zone: pre-publications, open archives (HAL, arXiv...), workshops
- Dark side: predatory publishers and fake conf.

In practice: a lot of back and forth (but one!)



So?

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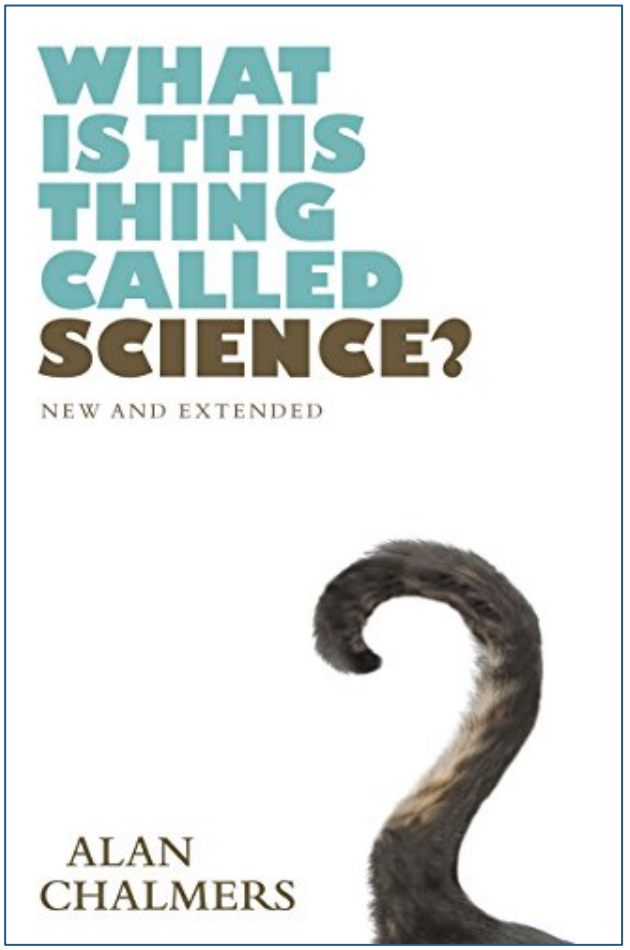

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Why Computational sciences?
...An why this course in 5IF ?

Why Computational sciences?
...An why this course in 5IF ?

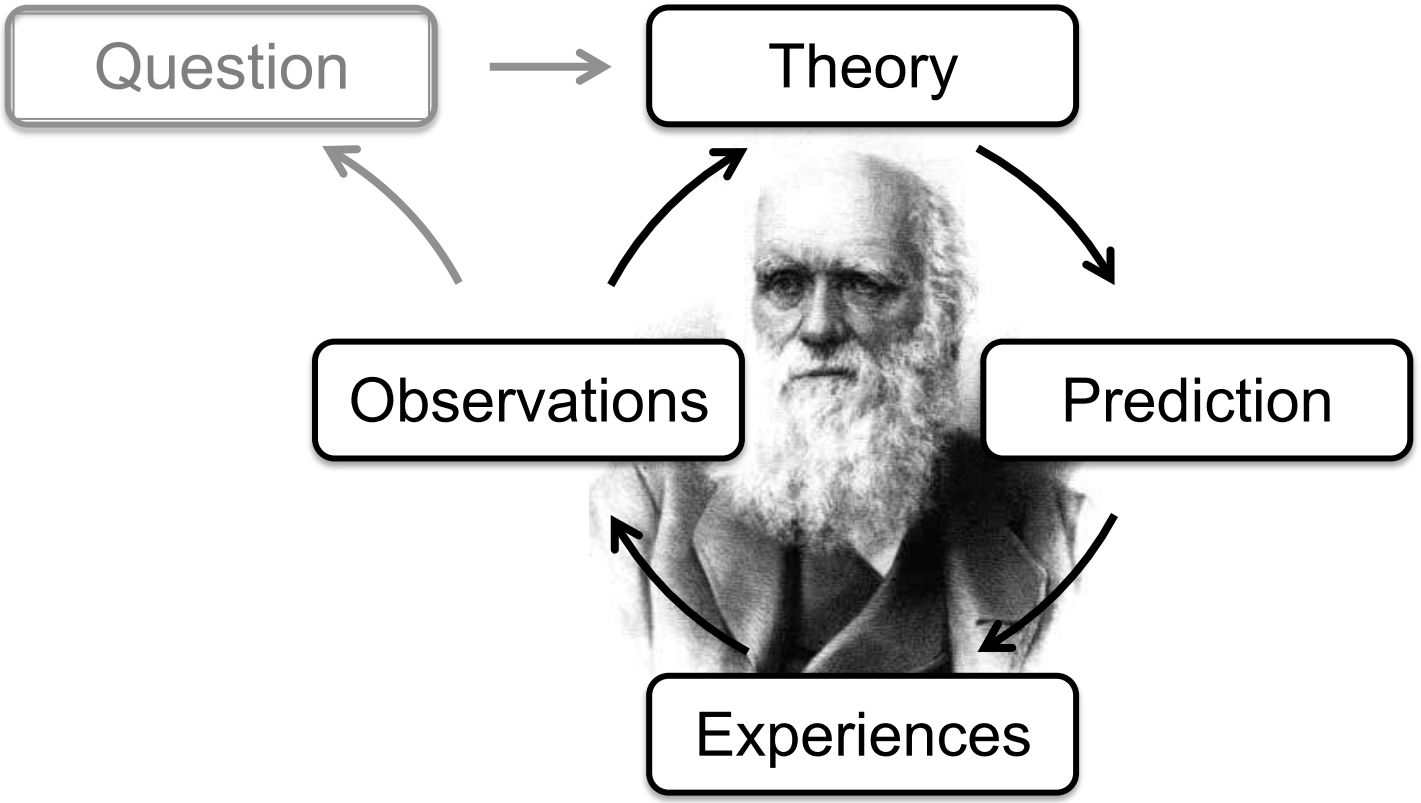
Because in 20 years everything has changed and we no longer do science "as we used to"!

Pourquoi les **sciences** computationnelles ?
...et pourquoi ce module en 5IF ?

Parce qu'en 10 ans tout à changé et qu'on ne fait plus de la science « comme avant » !

What changed?

- Historically, the "Theory-Observations" chain was entirely based on the scientist person, both in terms of deductions and observations...



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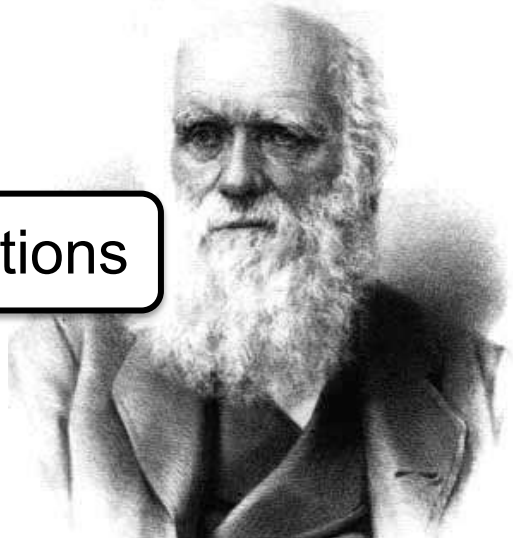
(2) Why are finches different?

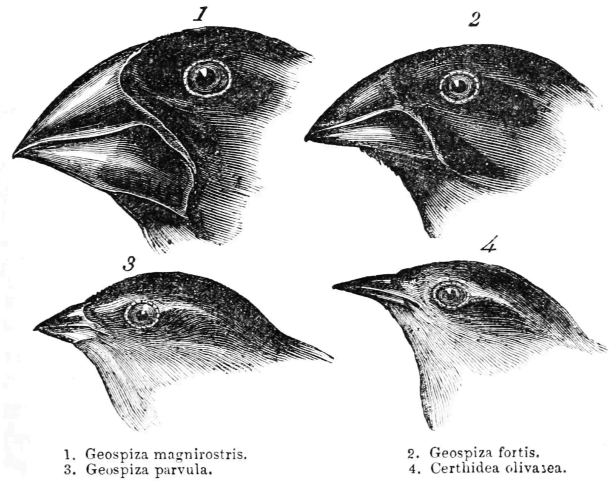
Question → Theory

(3) Evolution theory...

Observations



(1) 1835, Galapagos islands



1. Geospiza magnirostris.
3. Geospiza parvula.
2. Geospiza fortis.
4. Certhidea olivacea.

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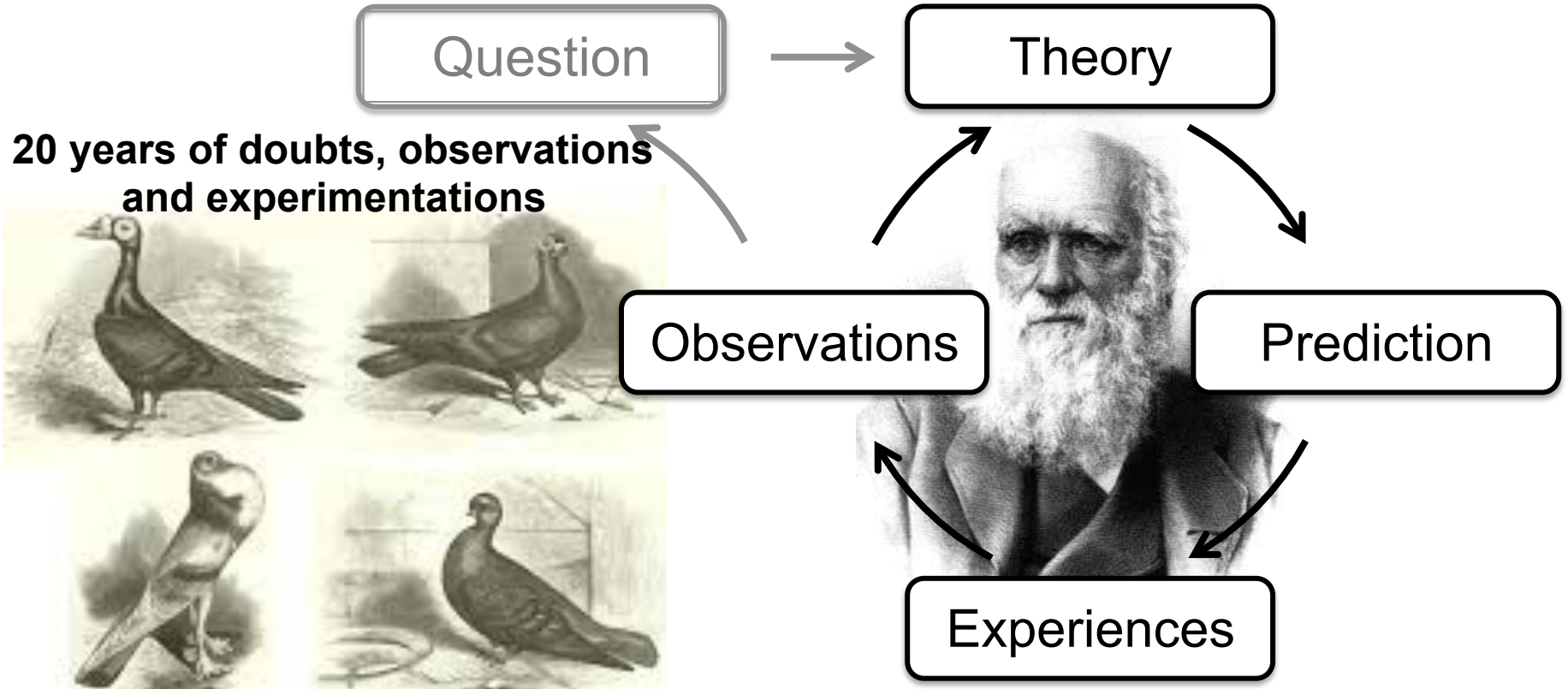

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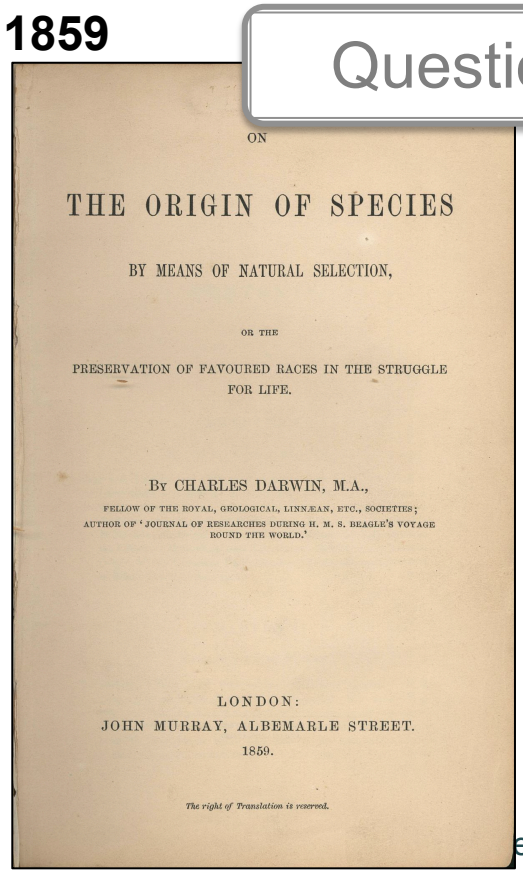
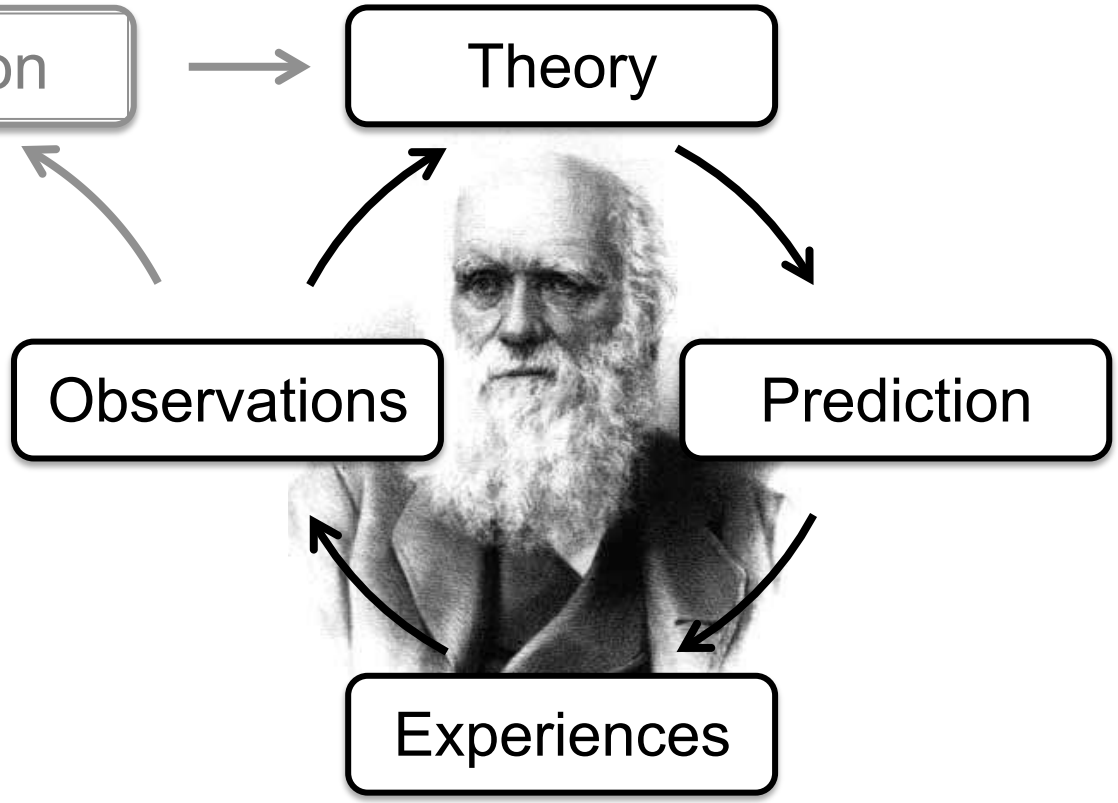
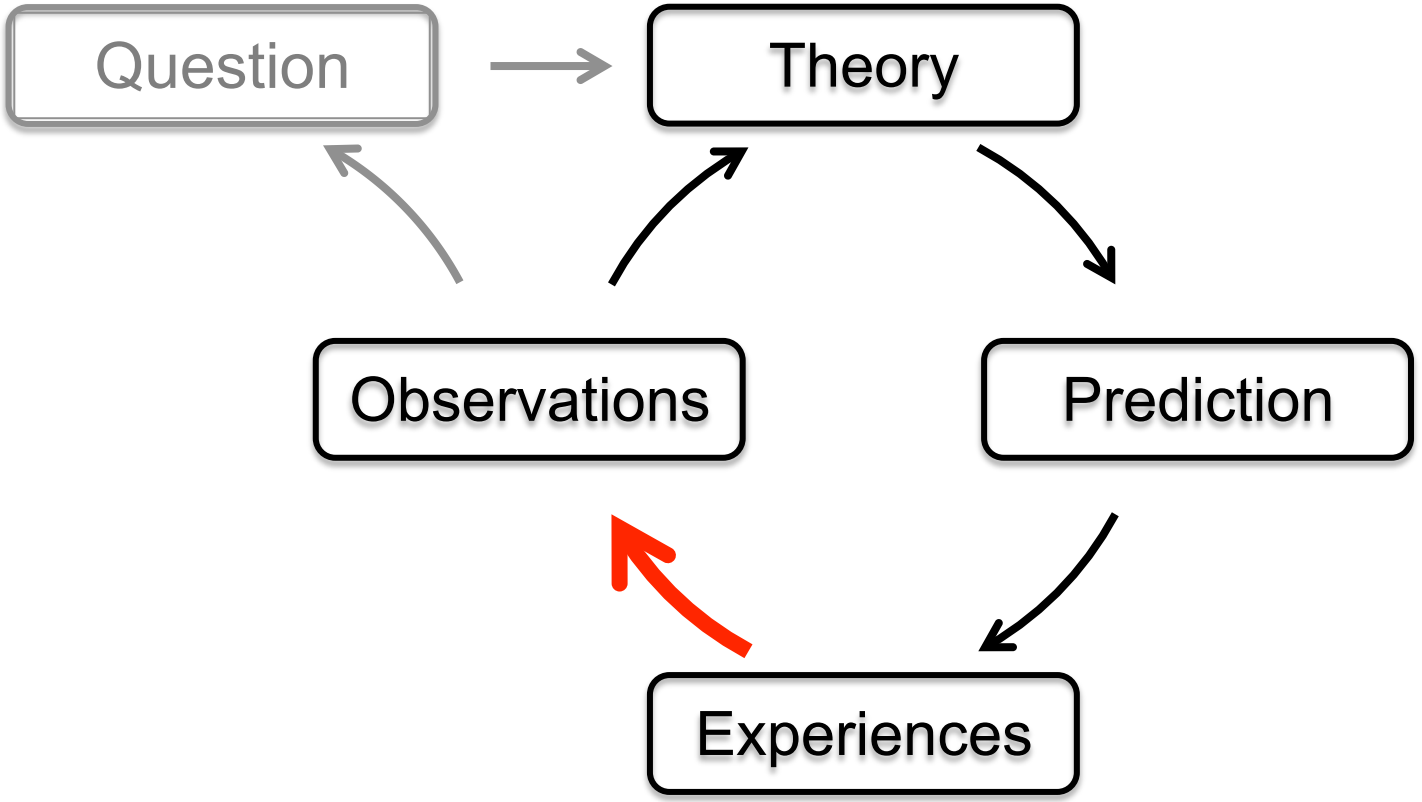




What changed?

1. Direct observation of experience has become the exception; experiences are “all” mediated by digital recording



Example (1) :

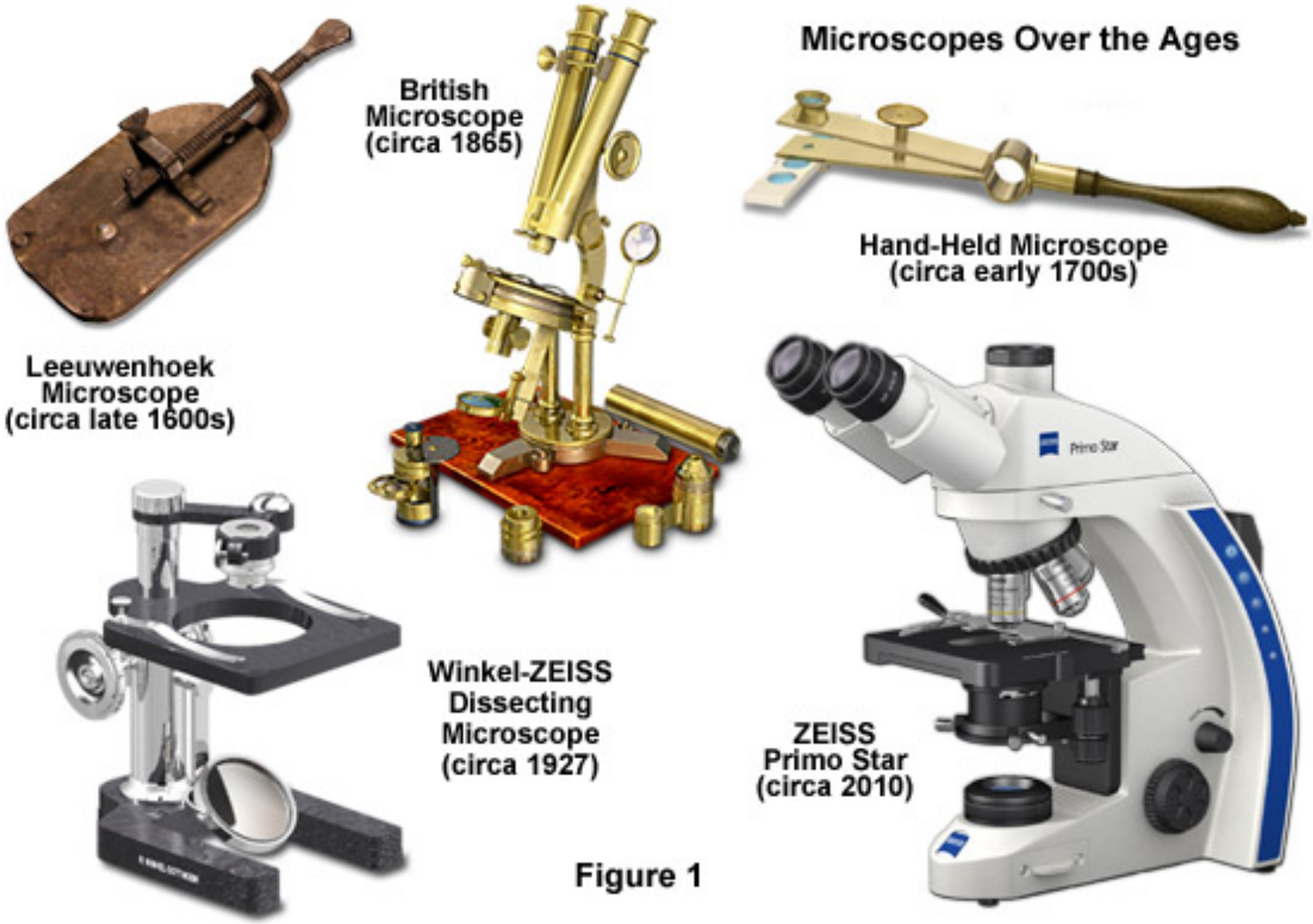


Figure 1

SWIFT educational microscope (2020)

Example (2) :

Vera Rubin, 1948

Example (2) :

Vera Rubin, 1970

Vera Rubin observatory (Chili)

(Large Synoptic Survey Telescope)

Observatoire Vera Rubin (Chili)

(Large Synoptic Survey Telescope)

VLT (Chili)

VLT control room (Chili)

Stellina telescope (2020)

Consequence

- The addition of intermediates is not a novelty (e.g. photography)
- The novelty is (1) the absence of direct observation (2) the switch to a digital intermediate
- The addition of a digital intermediate increases the experimental possibilities
- The addition of a digital intermediate (partly) removes the subjectivity of the scientist

But

- Any intermediate leads to a modification of the "signal" (i.e. in this case the observations and therefore the results of the experiment)
- The digital intermediate must be reliable and the modifications of the "signal" must be known and integrated into the analysis of the observations

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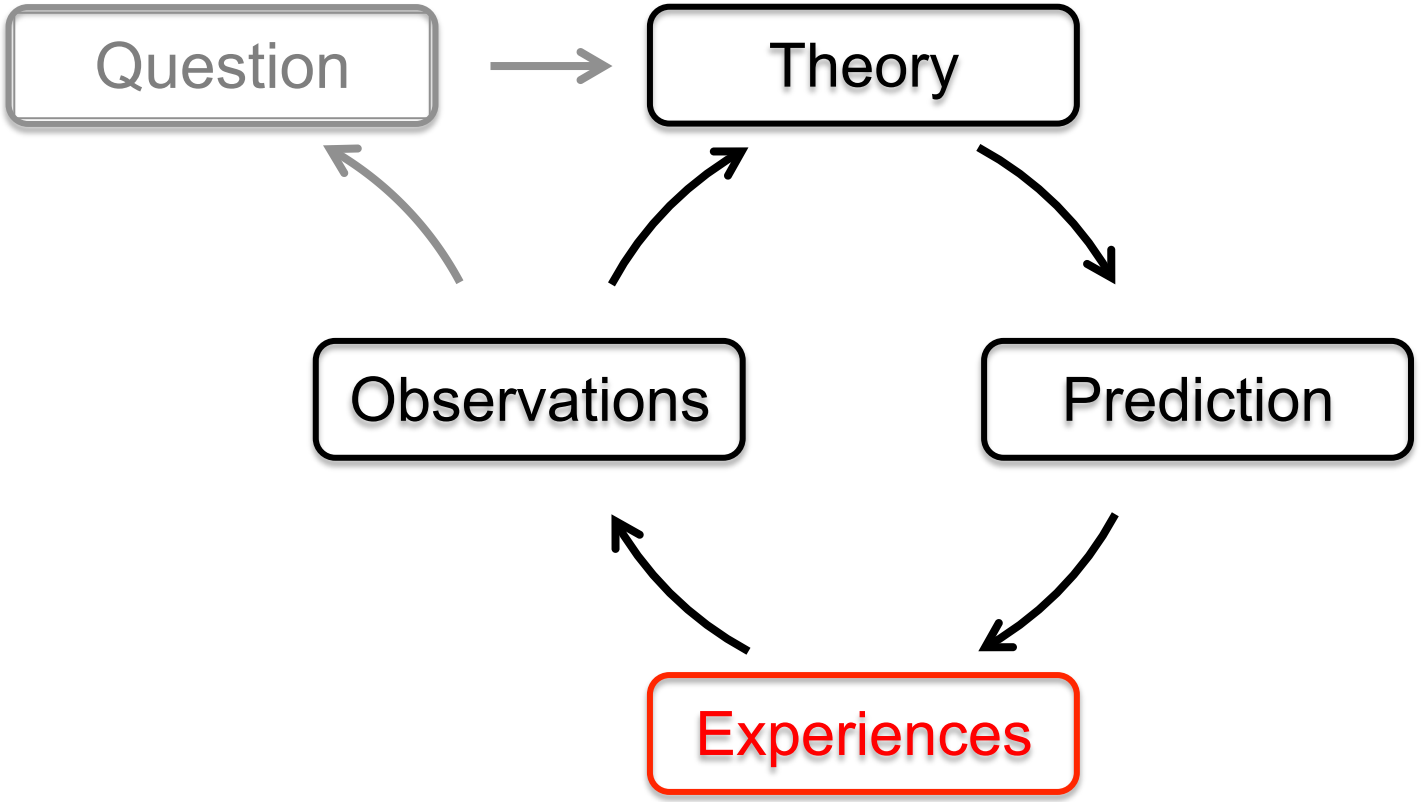
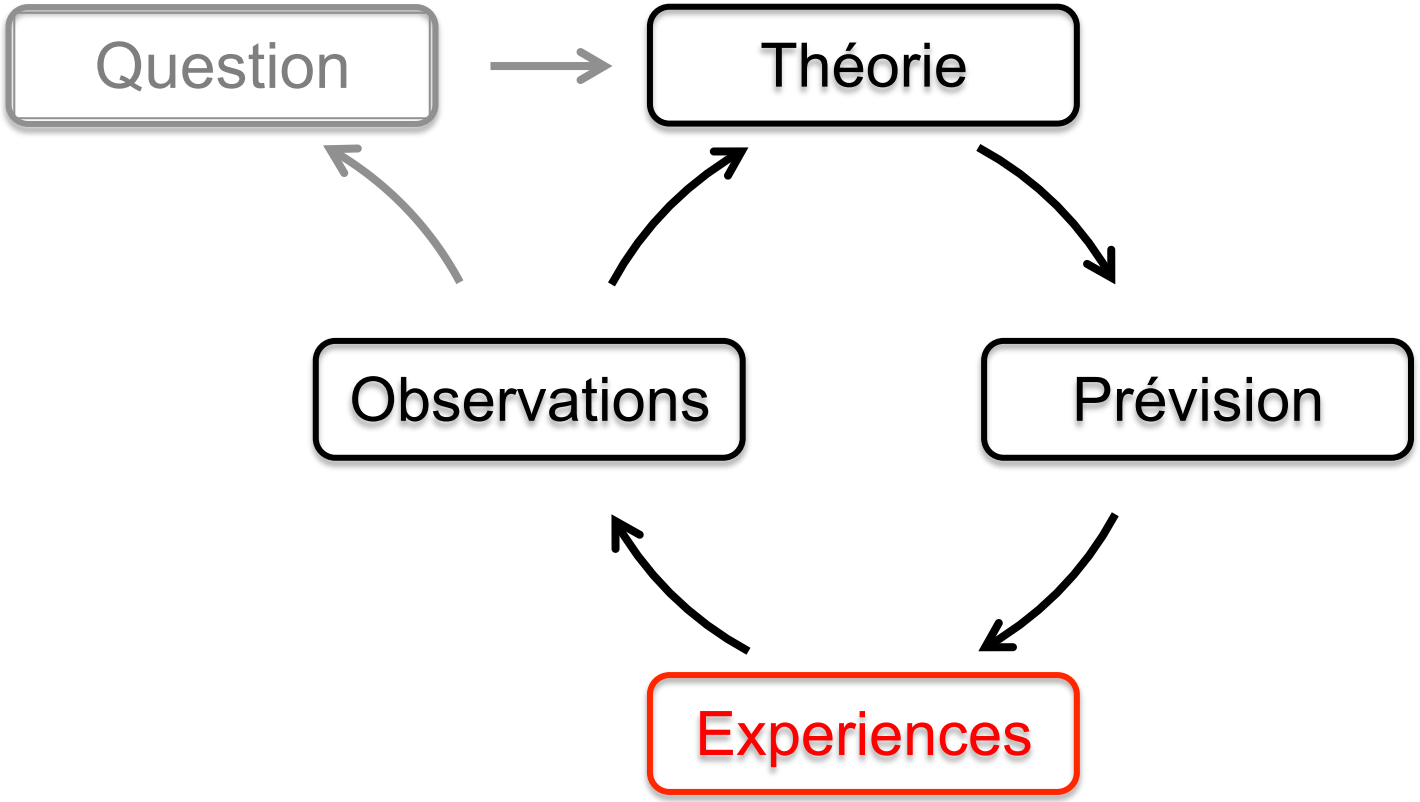


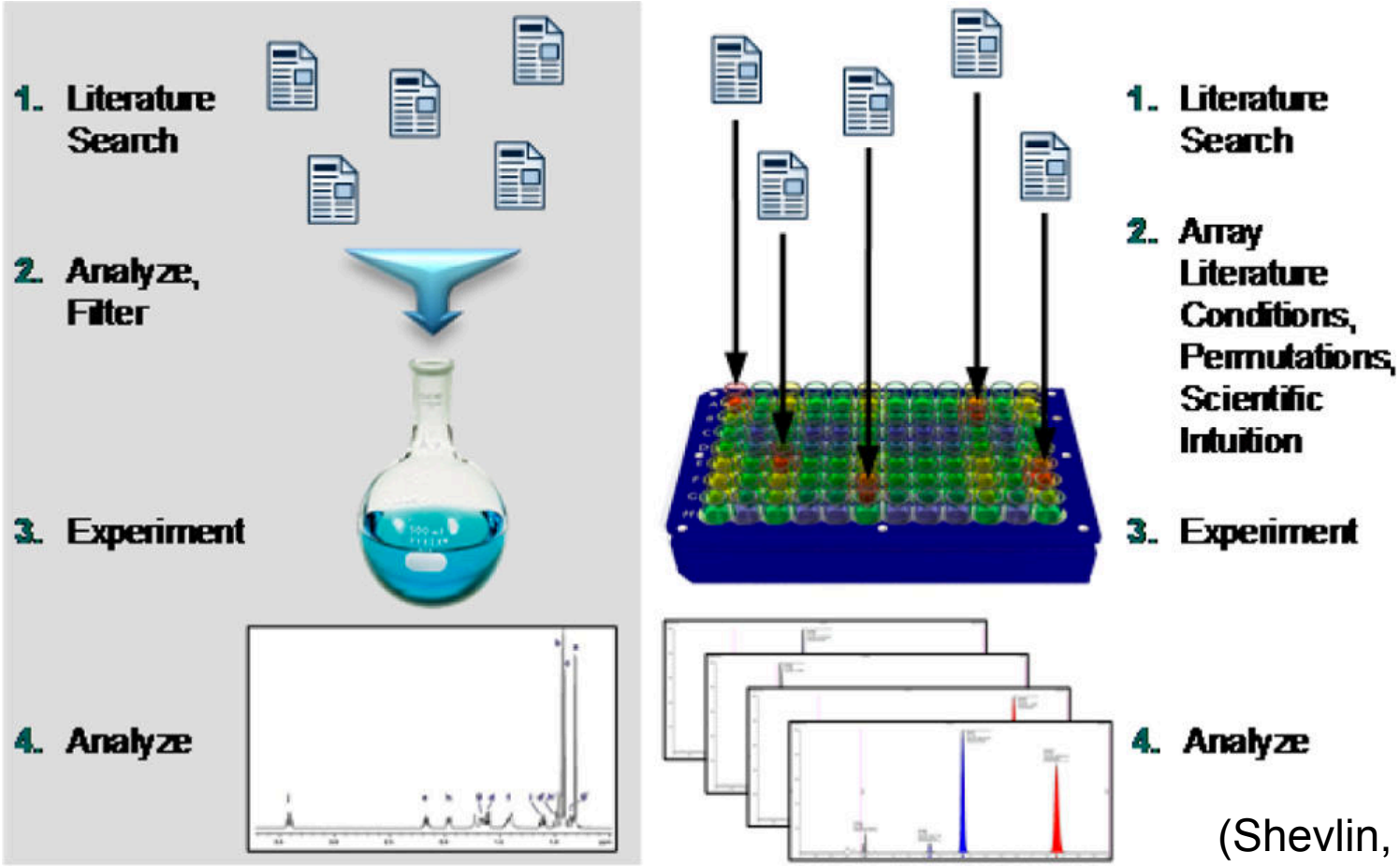
Qu’est-ce qui a changé ?

2. L’automatisation du recueil d’information entraine une explosion du volume des données scientifiques via la robotisation et la parallélisation des expériences



Les expériences « haut-débit »
(« High-Throughput experiments »)

- Expérimentation en parallèle et/ou en continu

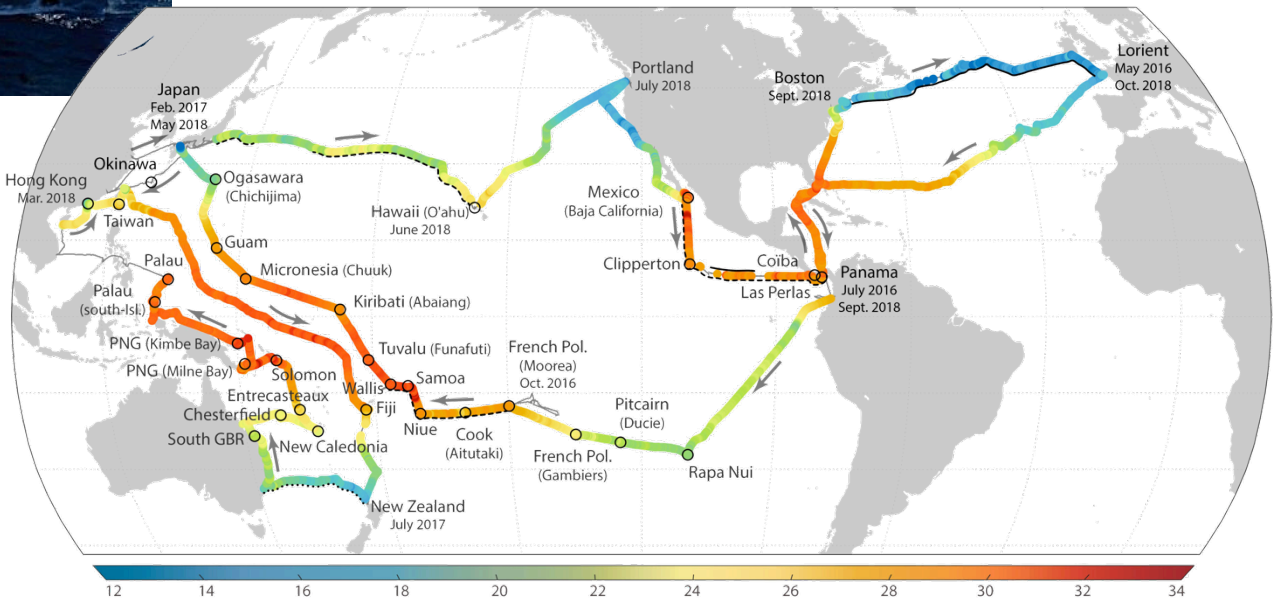


(Shevlin, 2017)

Exemple (1/2) : Tara Oceans

- 4 années de collecte
  - 210 points de collecte
- 35,000 échantillons d'« eau »
  - « Séquençage massif » des échantillons (méta-génomique)
  - « Phenotypage massif »

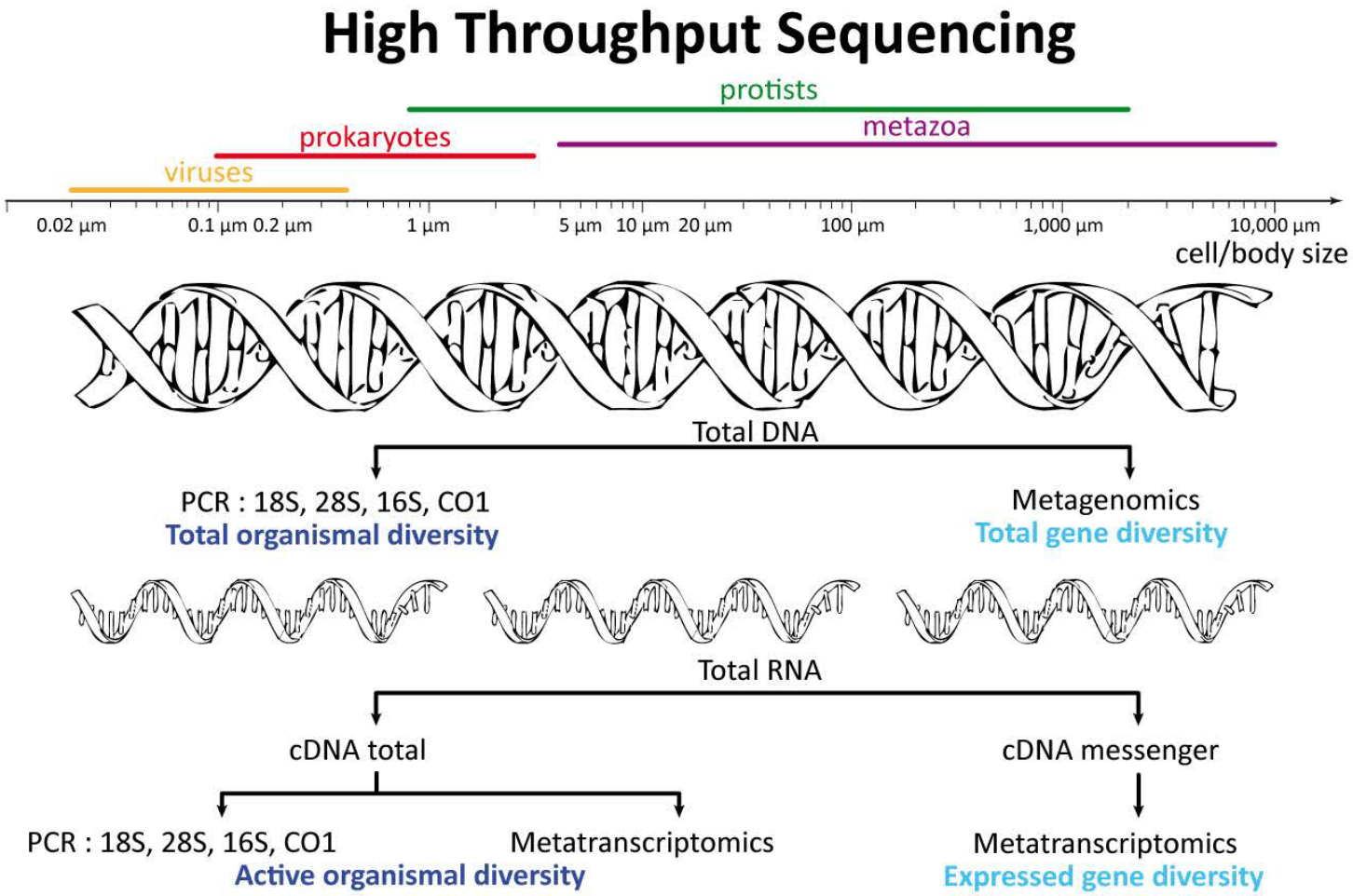
Le volume de données généré est impossible à estimer !



La « Data-Avalanche »

- Les données générées ont explosé
  - En Volume, en Variété, en Vélocité
  - Mais aussi en Accessibilité ...
- Tous les domaines scientifiques sont concernés ... Mais certains plus que d'autres !
  - Biologie (séquençage haut-débit, microscopie), écologie (télédétection), astronomie (capteurs ultra-haute définition), sciences de la terre (sismographes, télédétection, ...) ...
- L'avenir appartient à ceux qui pourront exploiter ces données
  - Stocker les données
  - Analyser les données
  - Croiser les données entre elles

Exemple (1/2) : Tara Oceans



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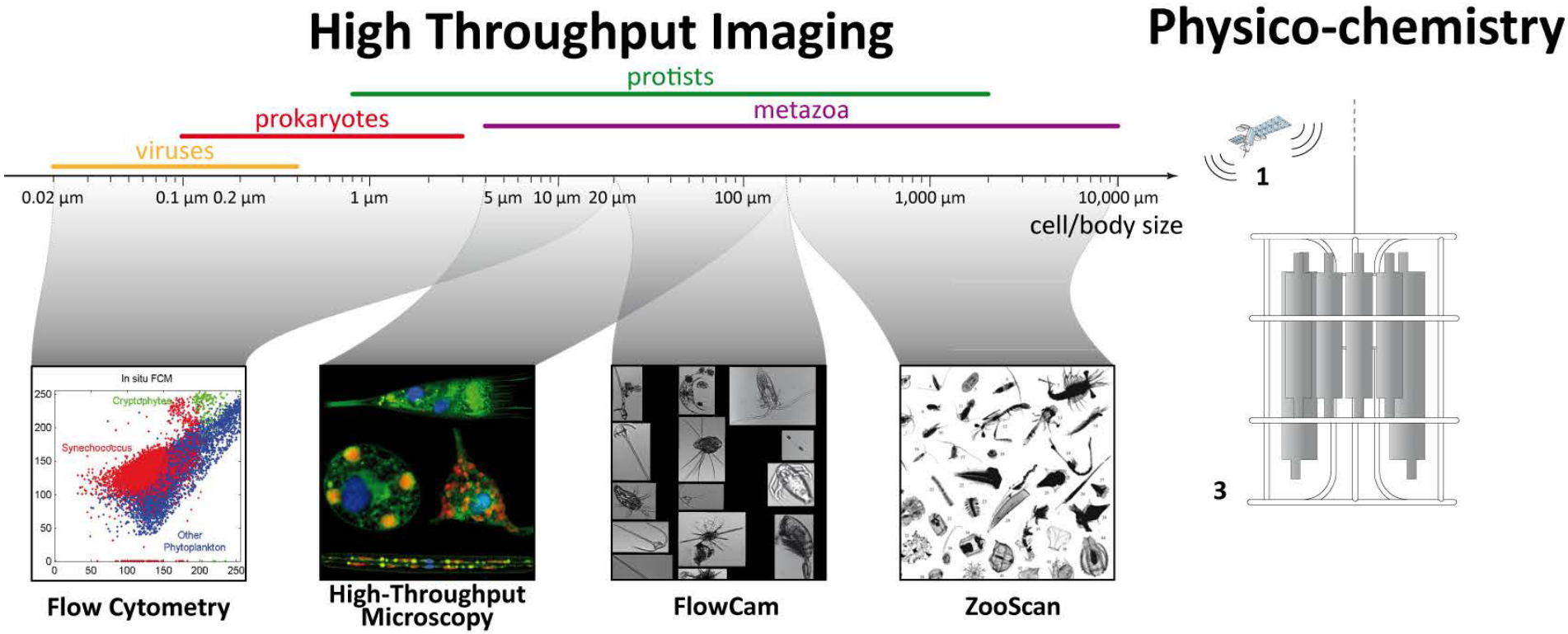
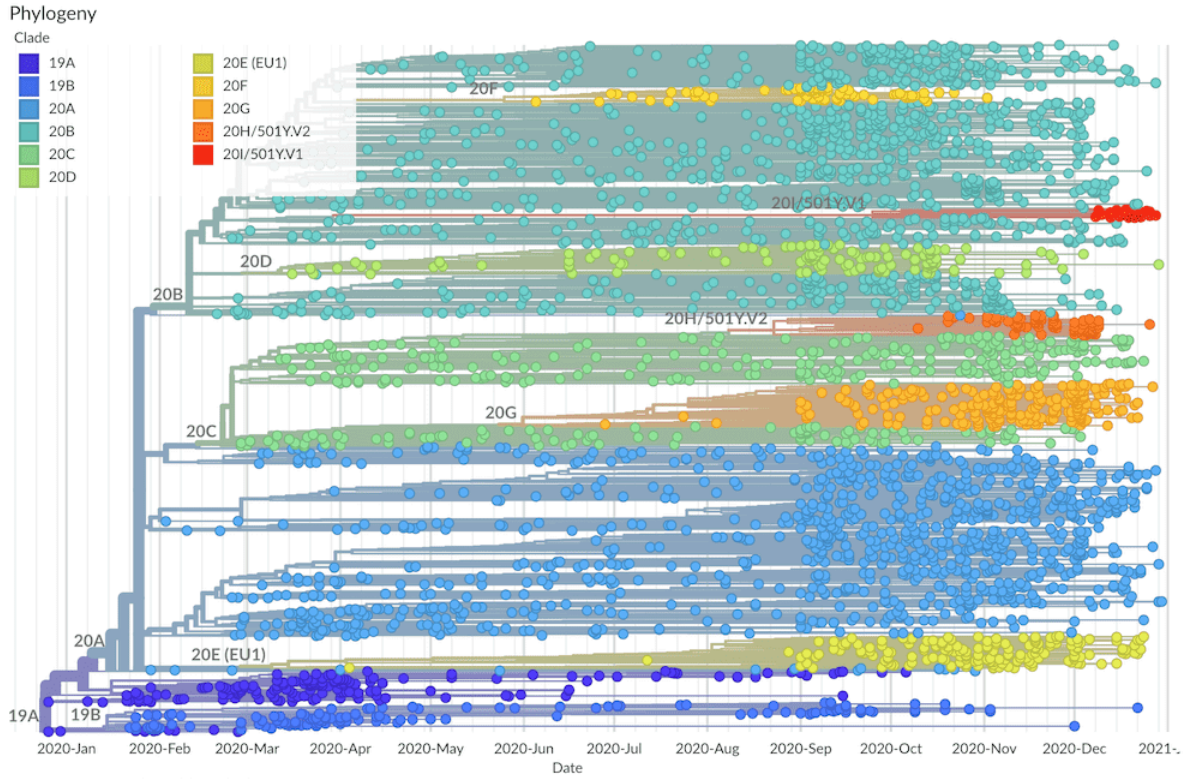
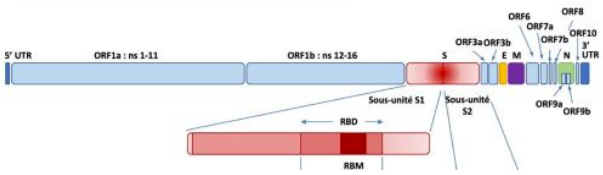


Exemple(2/2) : SARS-CoV-2

- Arbre phylogénétique de l'évolution du SARS-CoV-2 de janvier 2020 à janvier 2021 (Nextrain.org)
- En avril 2021, plus d'un million de séquences du SARS-CoV-2 étaient disponibles dans les bases de données ...





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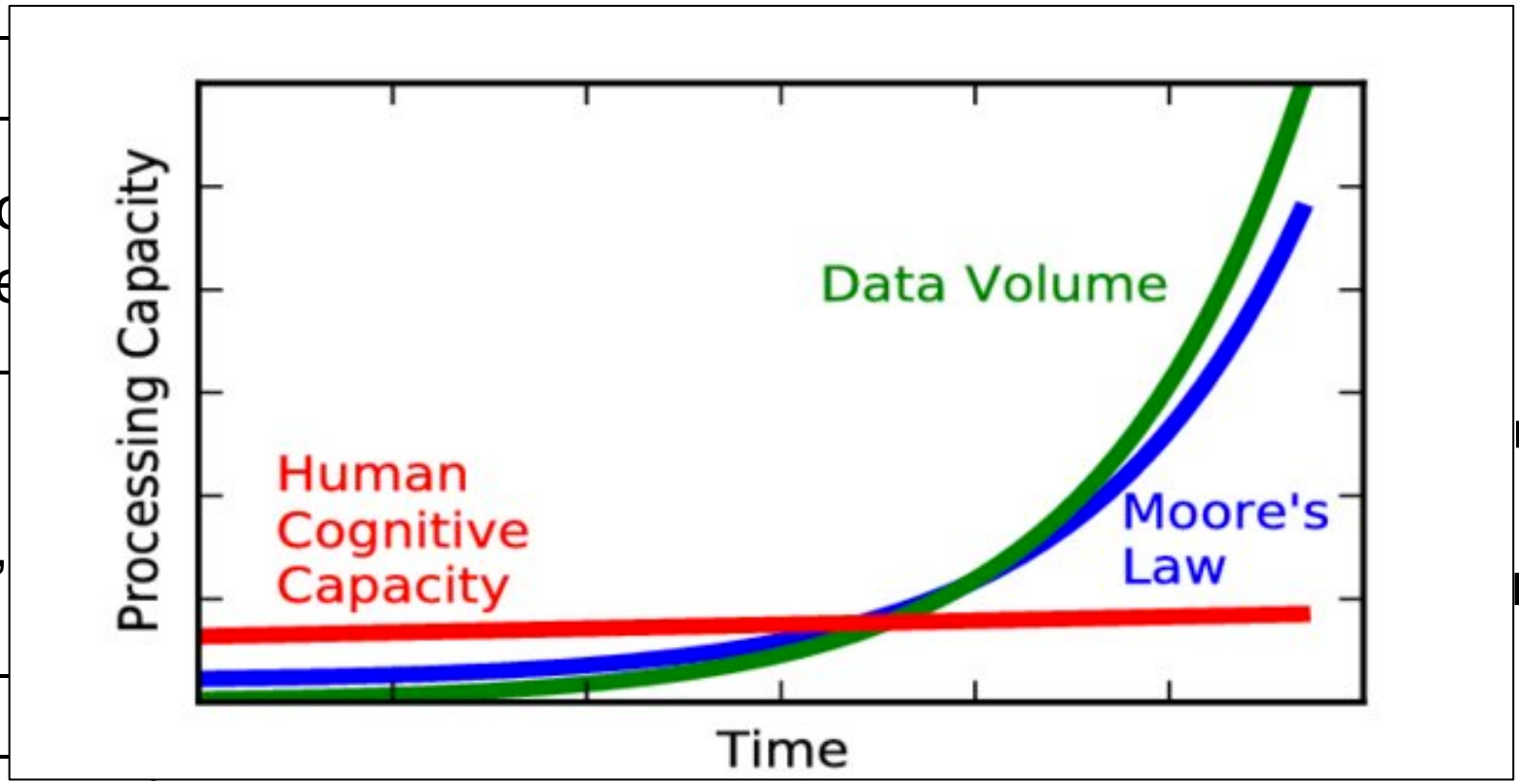

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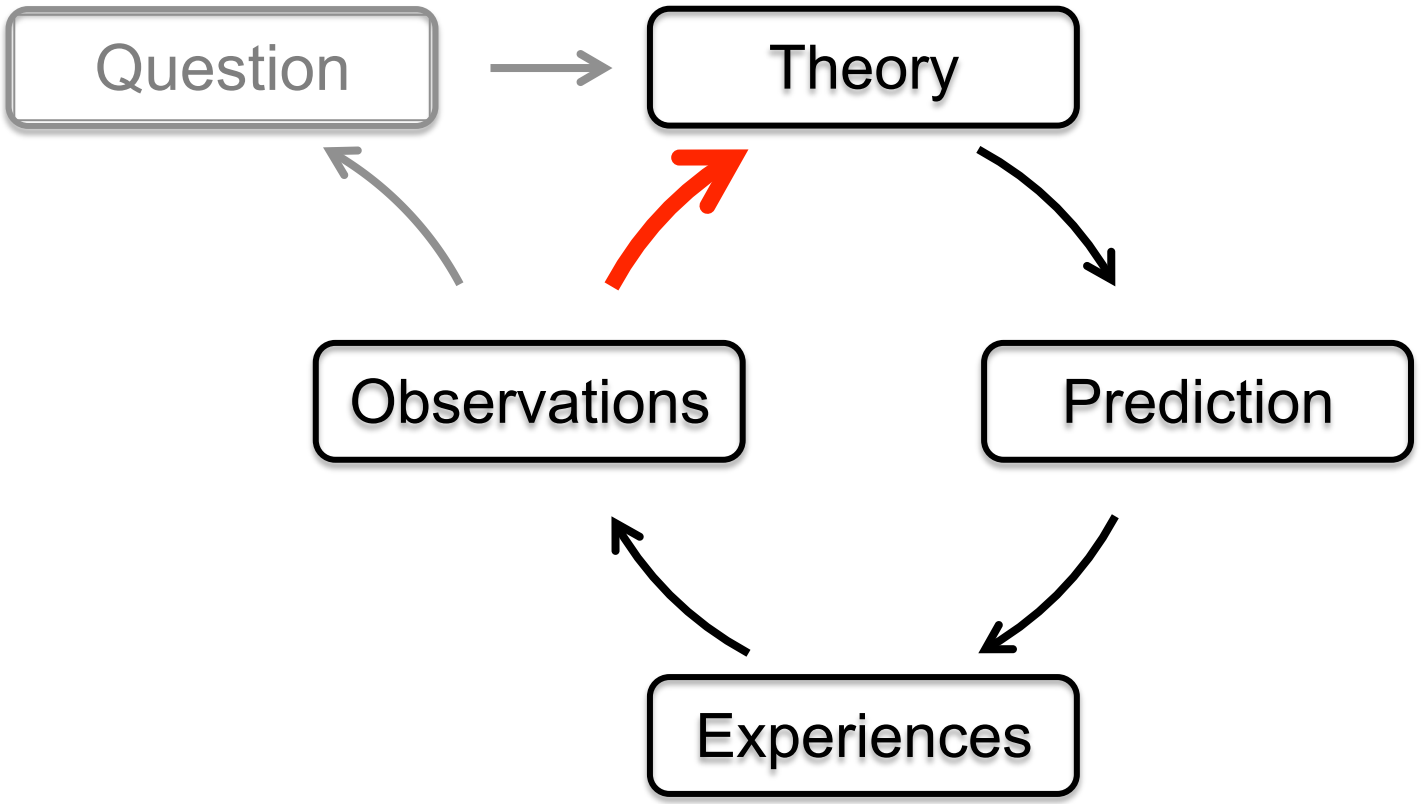
nées

  - Croiser les données entre elles

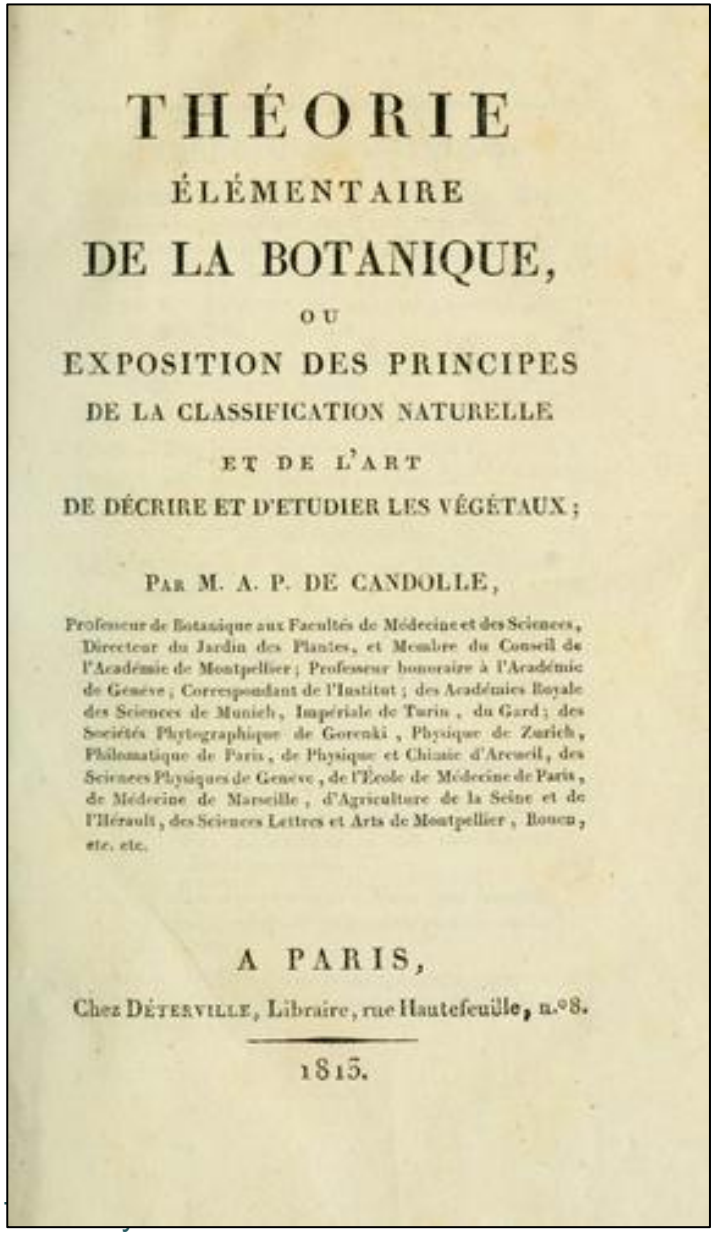
What changed?

3. The analysis of observations is increasingly assisted by mathematical and computer tools



Example (1) :

Augustin Pyramus de Candolle (1778-1841)



THÉORIE

ÉLÉMENTAIRE

DE LA BOTANIQUE,

OU

EXPOSITION DES PRINCIPES

DE LA CLASSIFICATION NATURELLE

ET DE L'ART

DE DÉCRIRE ET D'ETUDIER LES VÉGÉTAUX;

PAR M. A. P. DE CANDOLLE,

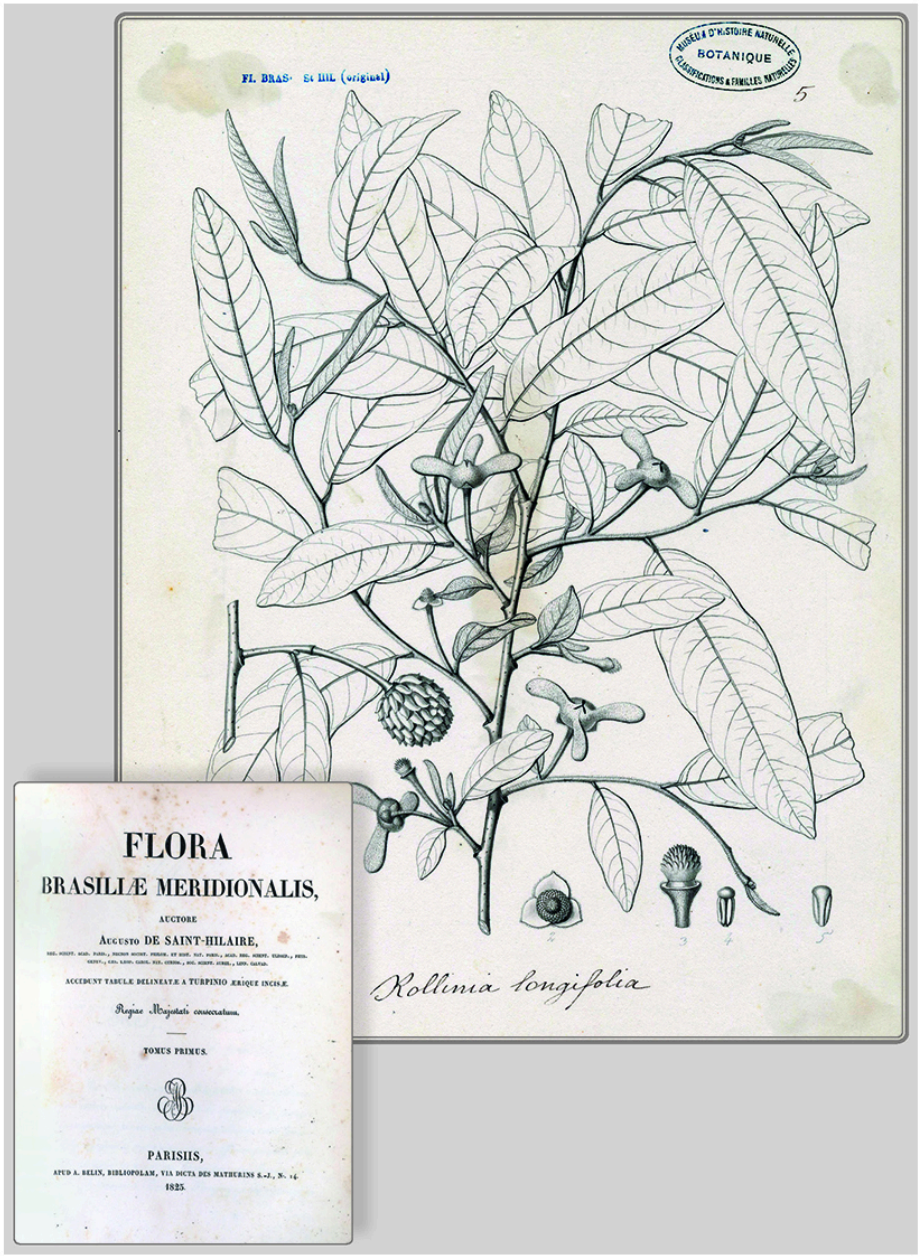
Professeur de Botanique aux Facultés de Médecine et des Sciences, Directeur du Jardin des Plantes, et Membre du Conseil de l'Académie de Montpellier; Professeur honoraire à l'Académie de Genève; Correspondant de l'Institut; des Académies Royale des Sciences de Munich, Impériale de Turin, du Gard; des Sociétés Phytographique de Gorenki, Physique de Zurich, Philomatique de Paris, de Physique et Chimie d'Arcueil, des Sciences Physiques de Genève, de l'École de Médecine de Paris, de Médecine de Marseille, d'Agriculture de la Seine et de l'Hérault, des Sciences Lettres et Arts de Montpellier, Rouen, etc. etc.

A PARIS,

Chez DÉTERVILLE, Libraire, rue Hautefeuille, n.°8.

1813.

Example (1) :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Rollinia longifolia
FLORA
BRASILLÆ MERIDIONALIS,
AUCTORE
Augusto DE SAINT-HILAIRE,
ACCEDUNT TABULÆ DELINEATÆ A TURPINIO ÆRIQUE INCISÆ.
Regiæ Majestati consecratum.
TOMUS PRIMUS.
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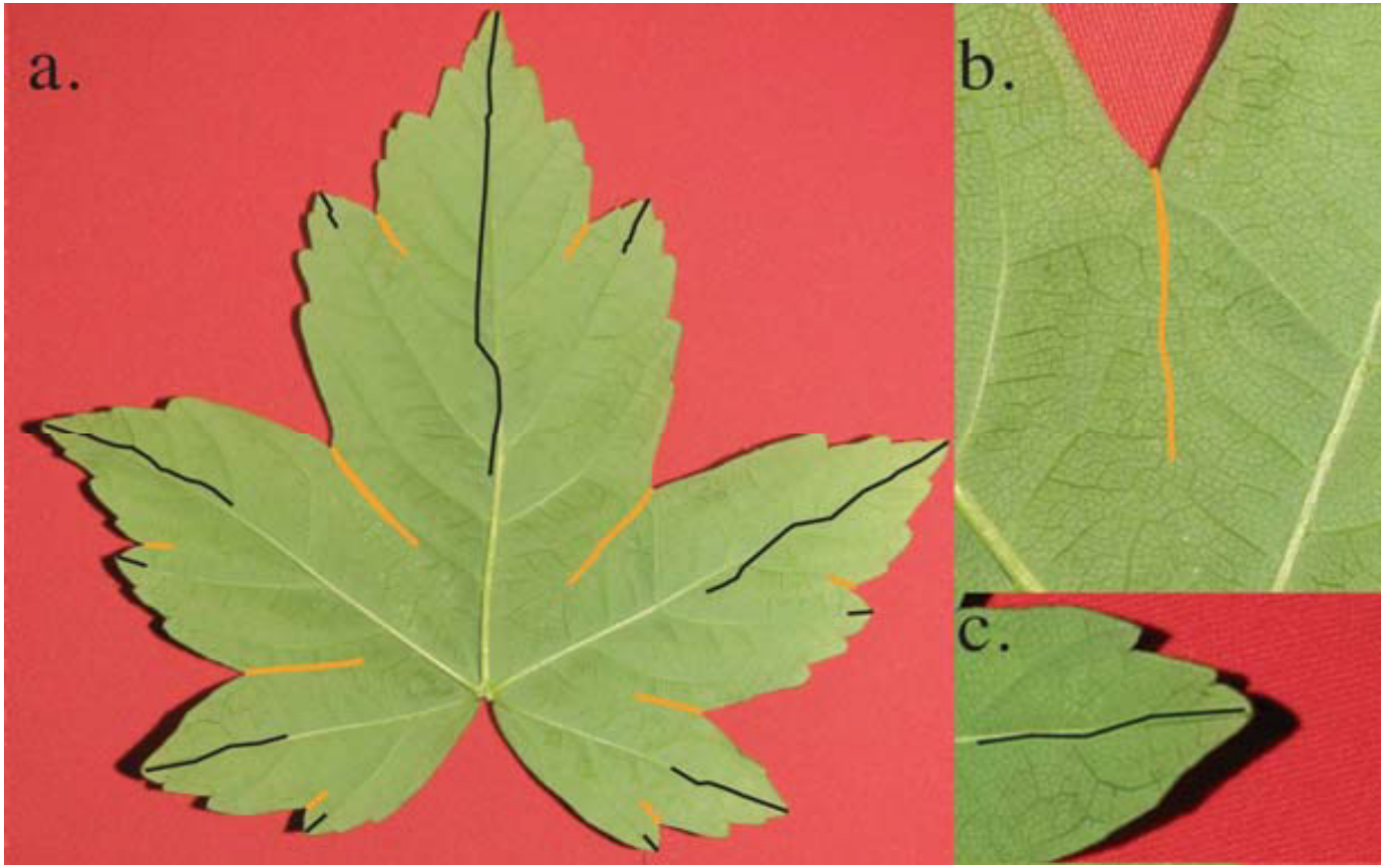
APUD A. BELIN, BIBLIOPOLAM, VIA DICTA DES MATHURINS S.-J., N. 14.
1825.

The filling law: a general framework for leaf folding and its consequences on leaf shape diversity

- Etienne Couturier, Sylvain Courrech Du Pont, Stéphane Douady, *Journal of theoretical biology, No.* 289, 2011



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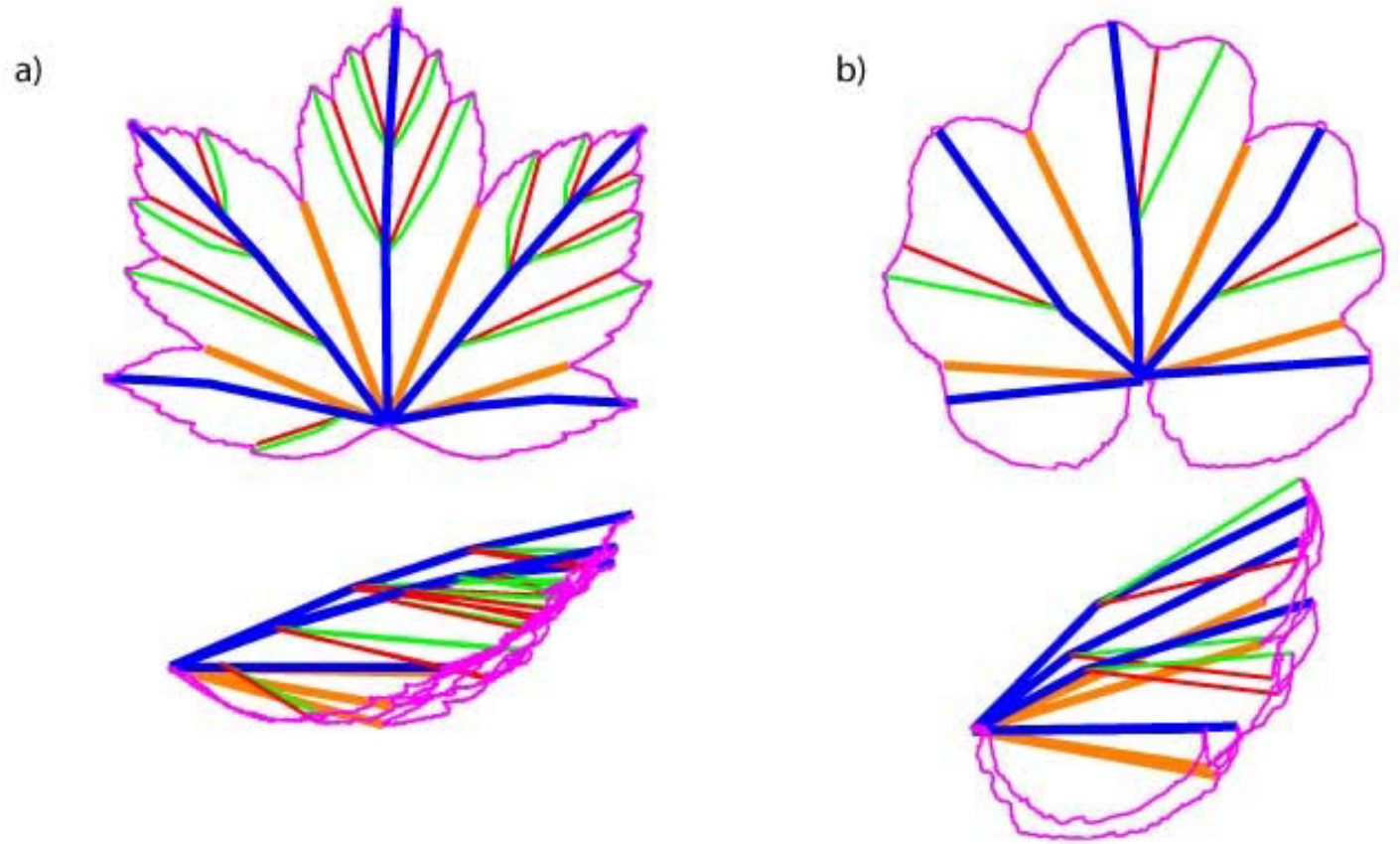

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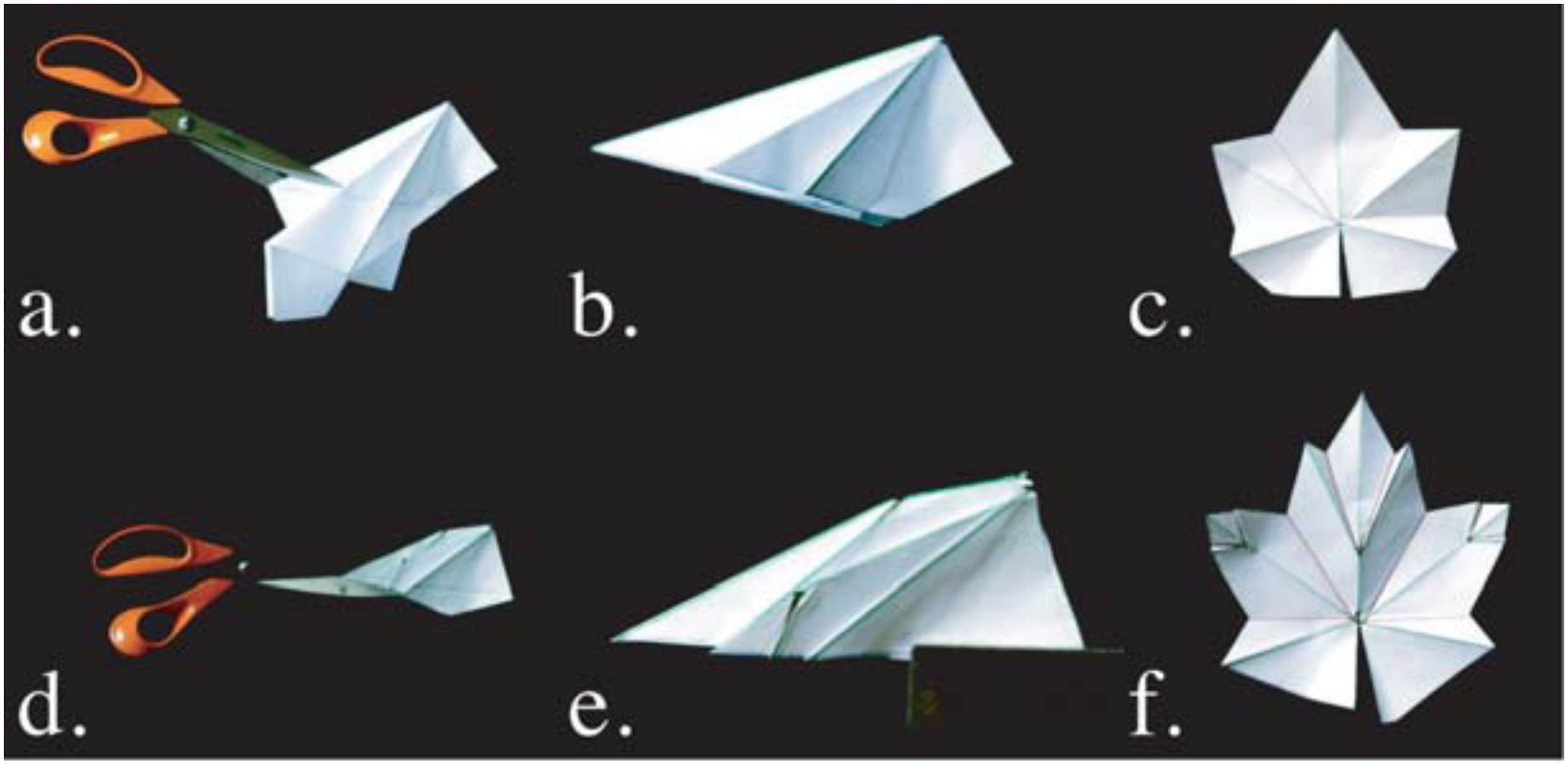

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Annex – Material and numerical folding methods

Material

Acer pseudoplatanus leaves were harvested in October or June in different gardens and forests in and around Paris, France. *Tetrapanax papyriferum* leaves come from our lab specimens, Pheonix Botanical garden in Nice, and Val Rahmeh Botanical garden in Menton. The buds of *Fagus sylvatica*, *Fagus sylvatica Rohan obelix* and *Ficus Carica* were collected in late spring in the Arboretum of Joinville-le-pont.

Numerical folding method

Leaves were numerically folded back using these drawing of their veins (synclinal folds), contour and anti-veins (anticlinal folds, Figure 26 a). For instance we took the picture of mature *Acer pseudoplatanus* or *Tetrapanax papyrifer* leaves. The main veins and secondary veins were drawn (by hand), acquiring the numerical positions. The contour was also acquired numerically.

frontiers in Plant Science

ORIGINAL RESEARCH
published: 2[illegible] June 2018
doi: 10.3389/fpls.2018.[illegible]

A Leaf Modeling and Multi-Scale Remeshing Method for Visual Computation via Hierarchical Parametric Vein and Margin Representation

Weiliang Wen[1,2], *Baojun Li*[3]*, *Bao-jun Li*[3] and *Xinyu Guo*[1,2]

[1] *Beijing Research Center for Information Technology in Agriculture, Beijing, China,* [2] *Beijing Key Lab of Digital Plant, National Engineering Research Center for Information Technology in Agriculture, Beijing, China,* [3] *Faculty of Vehicle Engineering and Mechanics, School of Automotive Engineering, Dalian University of Technology, Dalian, China*

This paper introduces a novel hierarchical structured representation for leaf modeling and proposes a corresponding multi-resolution remeshing method for large-scale visual computation. Leaf modeling is a very difficult and challenging problem due to the wide

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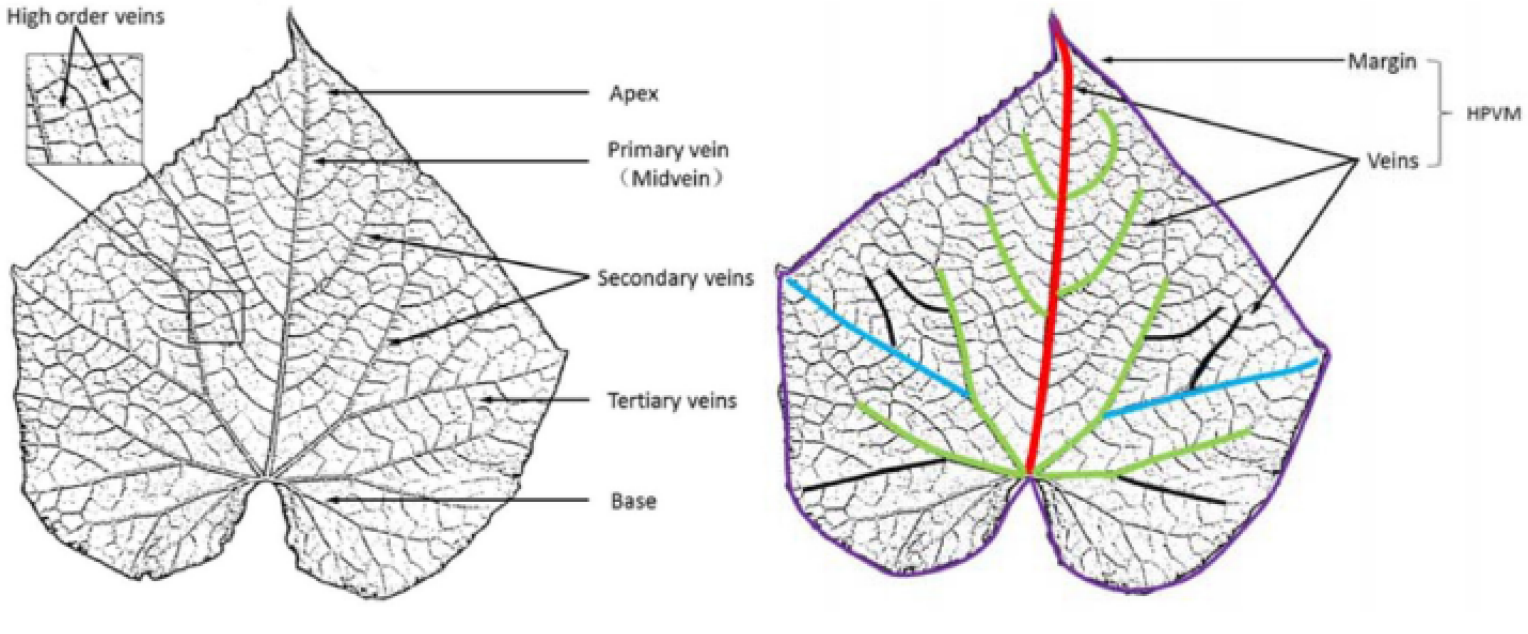

FIGURE 2 | HPVM model extraction of a real leaf. The colored curves denote different level veins and the leaf margin.

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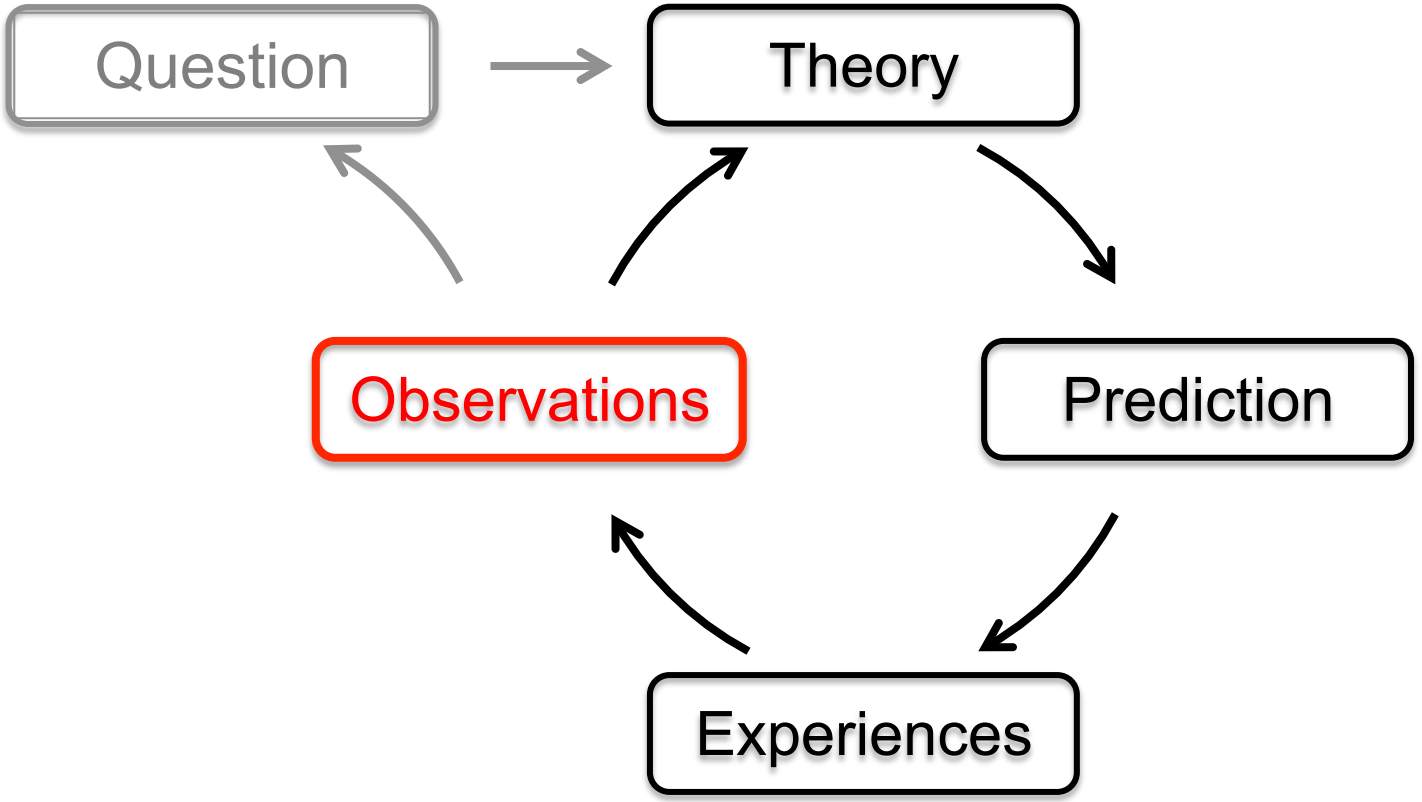
This paper introduces a novel hierarchical structured representation for leaf modeling and proposes a corresponding multi-resolution remeshing method for large-scale visual computation. Leaf modeling is a very difficult and challenging problem due to the wide

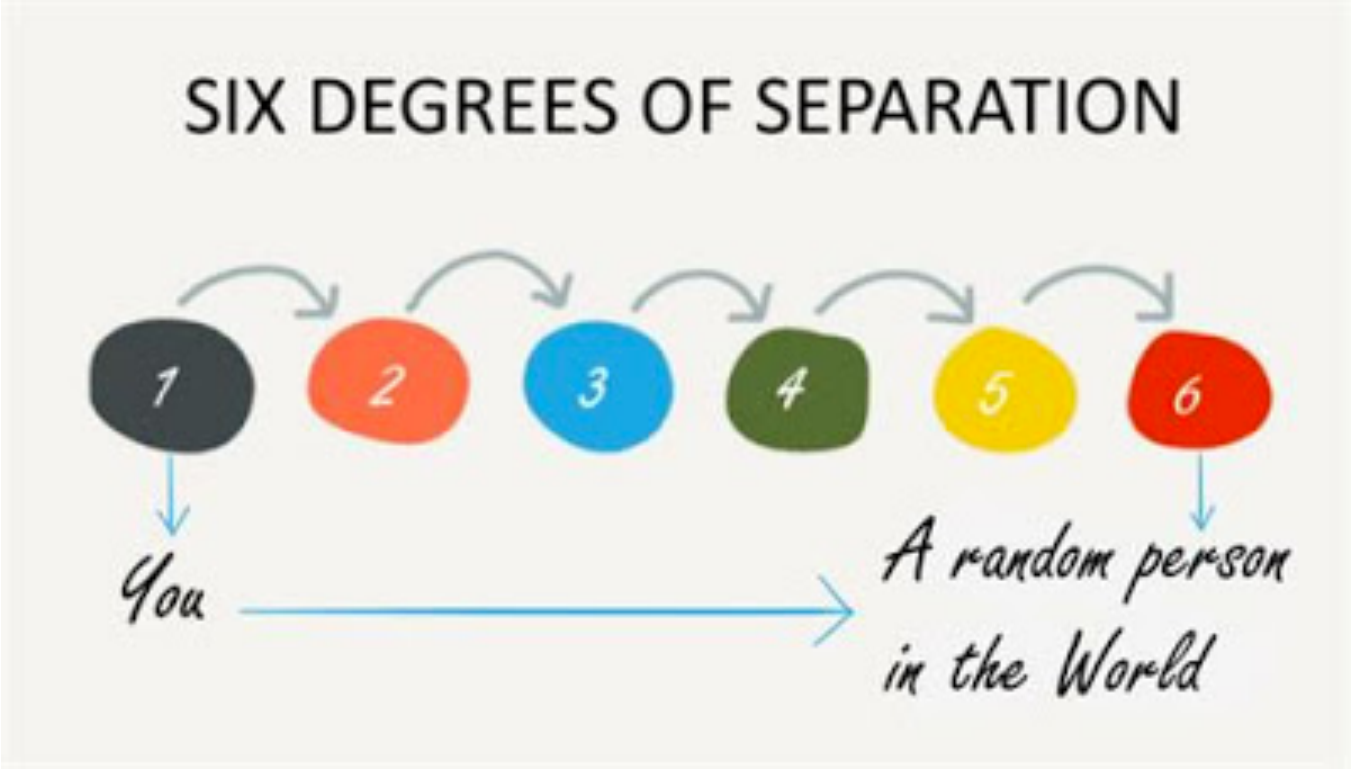
What changed?

4. The deployment of digital tools in all areas of society provides access to new observations ... On society!



Example

- Six degrees of separation
  - “theory” proposed in 1929 by Frigyes Karinthy (writer, poet, dramatist)



https://intheloop888.blogspot.com/

Six degrees of separation

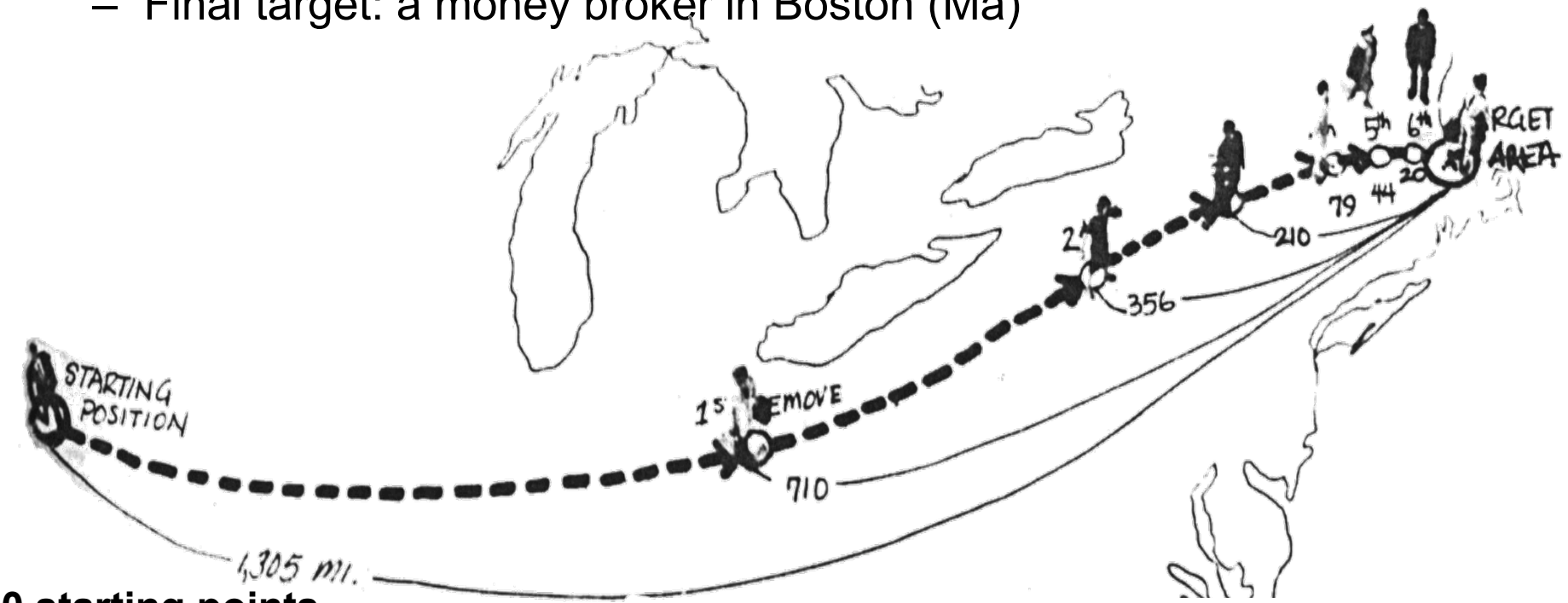
- How can such a theory be tested experimentally?

Stanley Milgram, 1967

(well known for his Experiment on Obedience)

Six degrees of separation

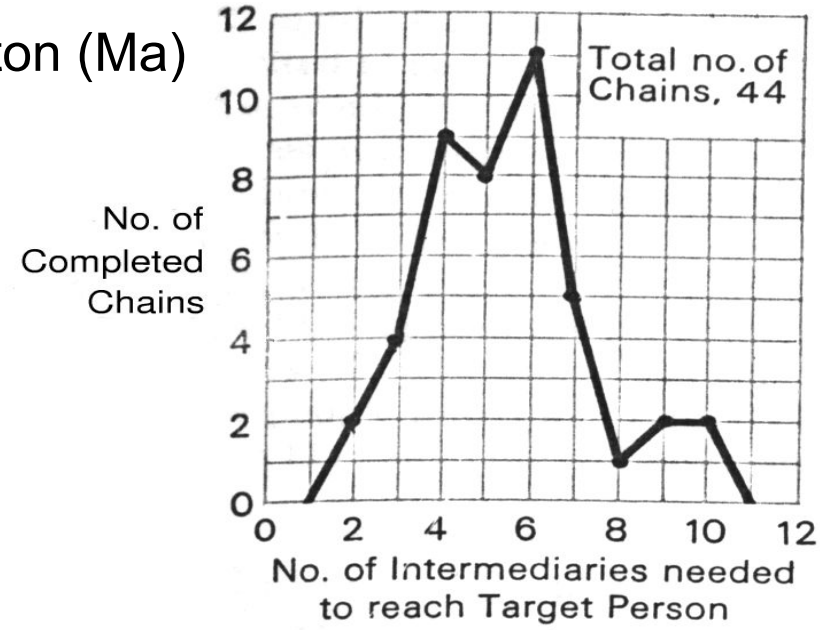
- How can such a theory be tested experimentally?
  - 160 letters hand-given to Omaha citizens (Nebraska)
  - Rule: send the letter to one of your acquaintance
  - Final target: a money broker in Boston (Ma)



[Stanley Milgram, 1967]

Six degrees of separation

- How can such a theory be tested experimentally?
  - 160 letters hand-given to Omaha citizens (Nebraska)
  - Rule: send the letter to one of your acquaintance
  - Final target: a money broker in Boston (Ma)
- Résults :
  - 44/160 letters arrived
  - Mean hop number: 5.43
  - Median hop number: 5
  - → « Six degrees of separation »
  - → « Small-World » model: $l \sim \log N$

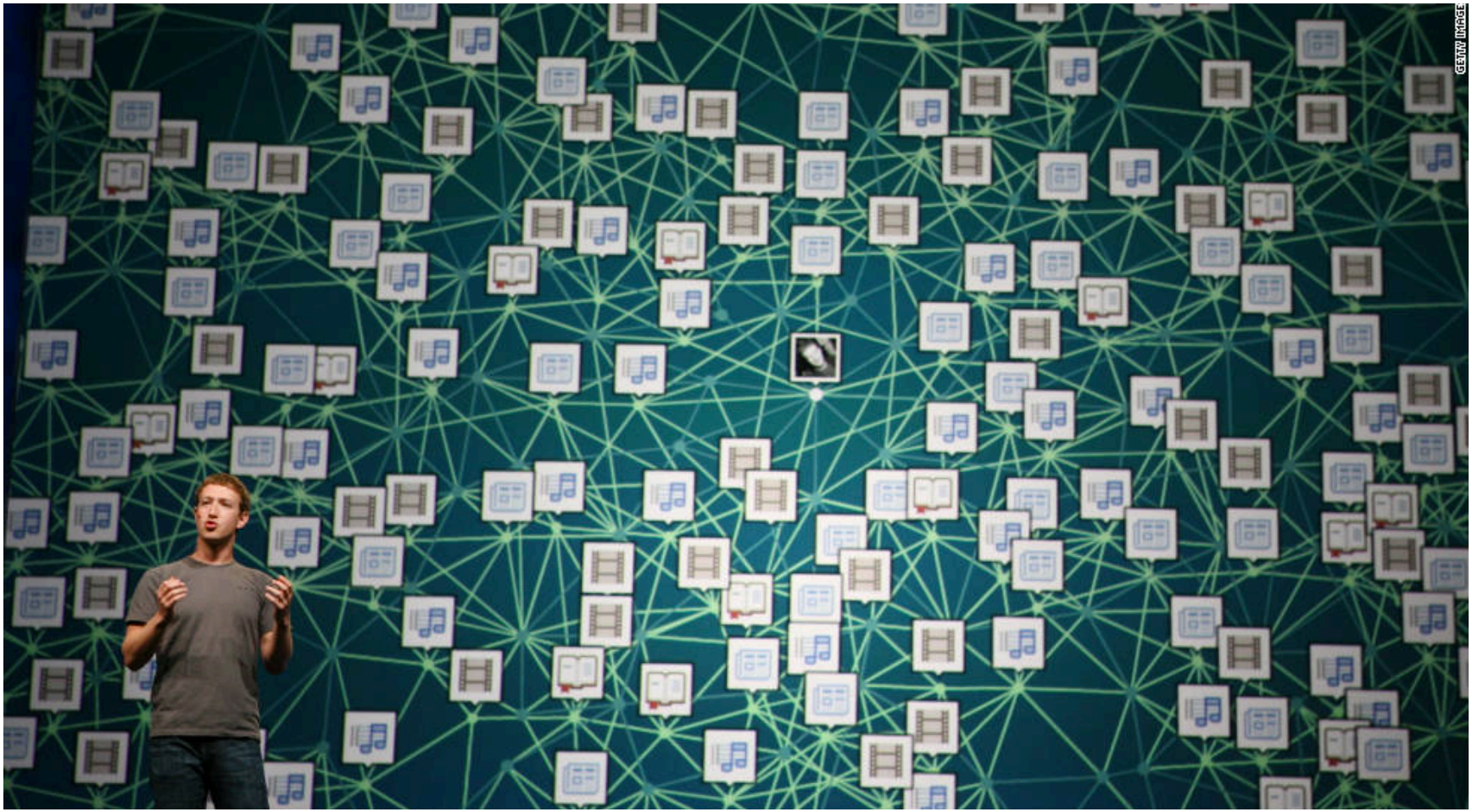


In the Nebraska Study the chains varied from two to 10 intermediate acquaintances with the median at five.

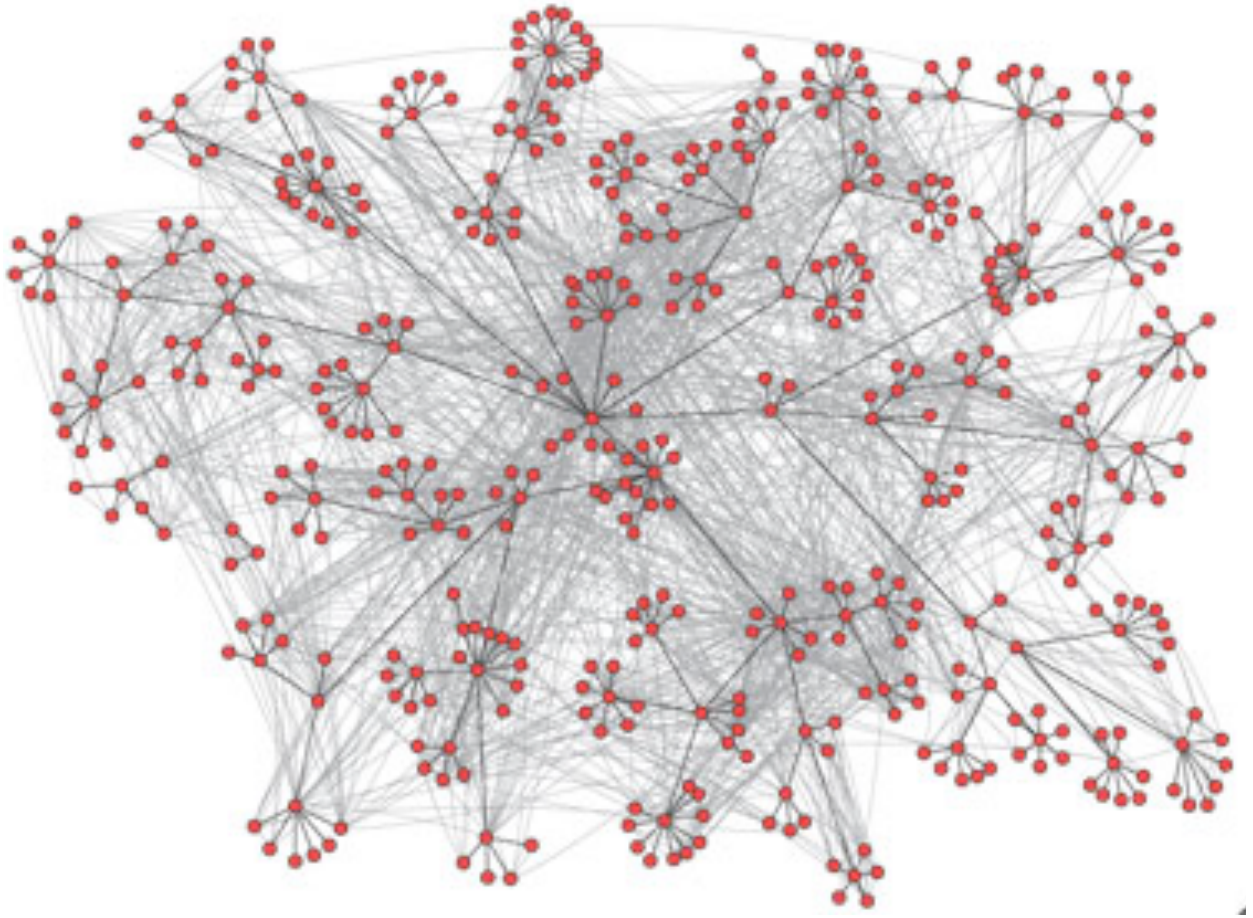
[Stanley Milgram, 1967]

Six degrees of separation...
...in the digital world!

“On Facebook, it's now 4.74 degrees of separation” (CNN 2011)



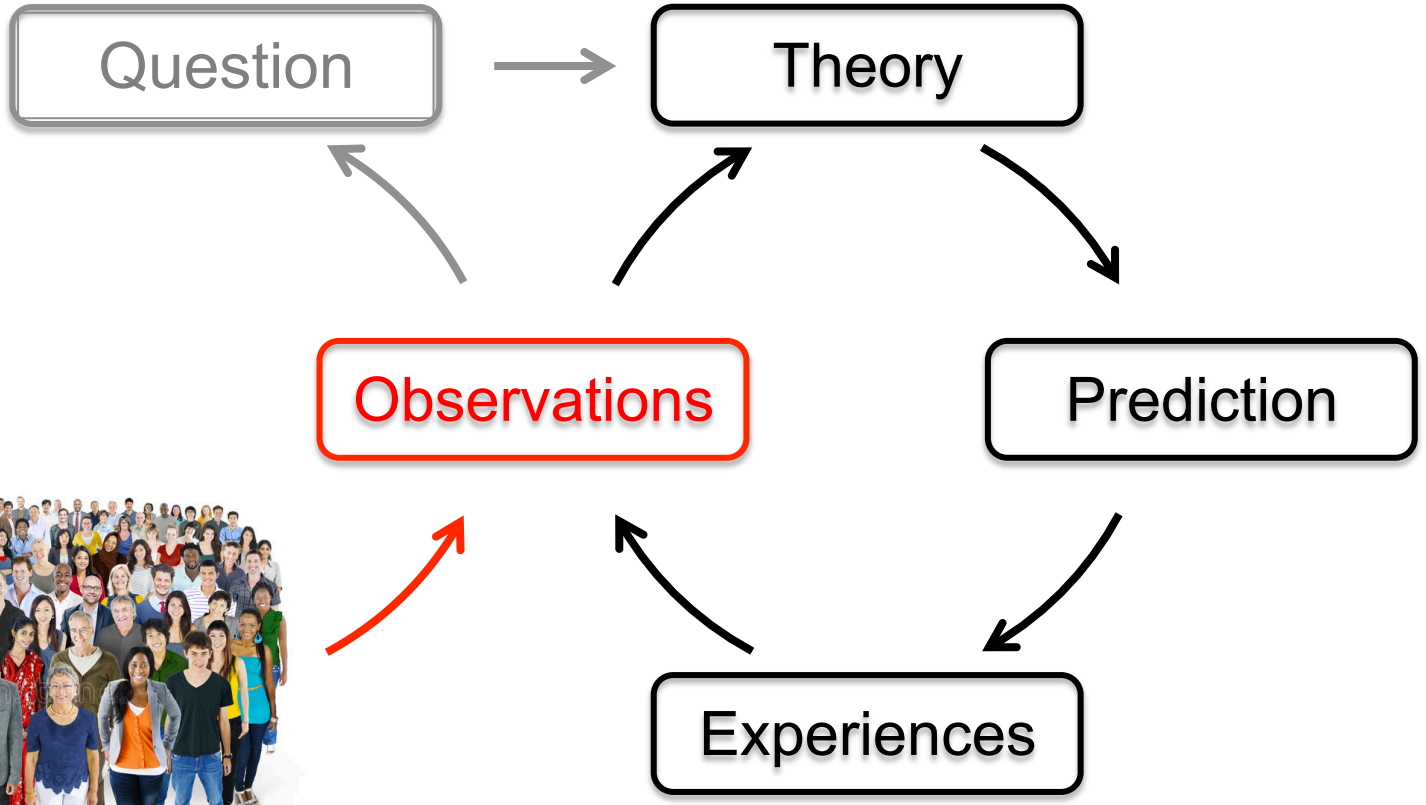
Digitalization of communications shed a new light on social systems...



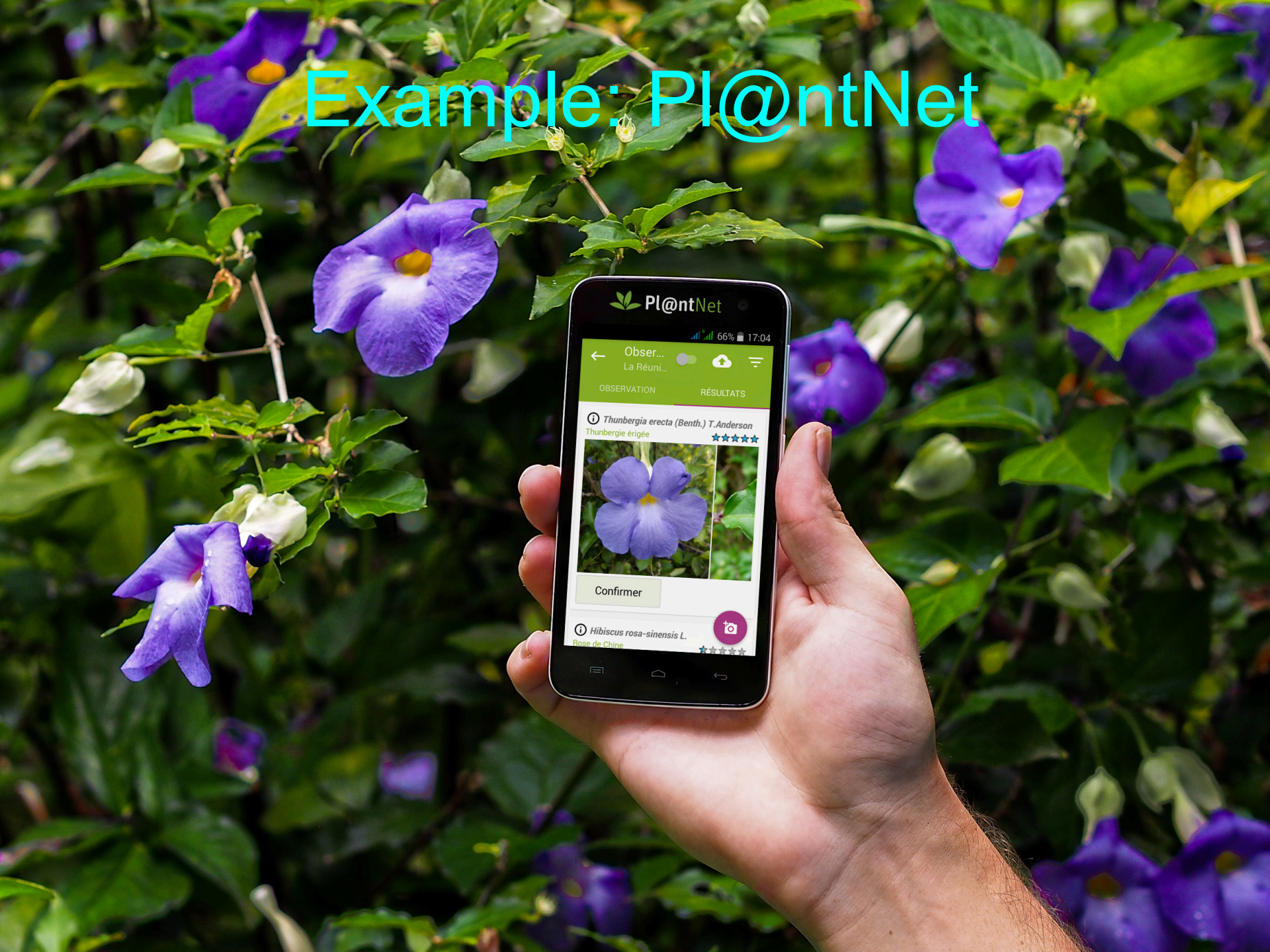
Mails exchanged between 436 employees of Hewlett-Packard Research Lab. compared to the hierarchical structure of the lab.

What changed?

5. The democratisation of digital tools (computers, telephones) allows the general public to participate in large-scale scientific projects
→ Participatory science



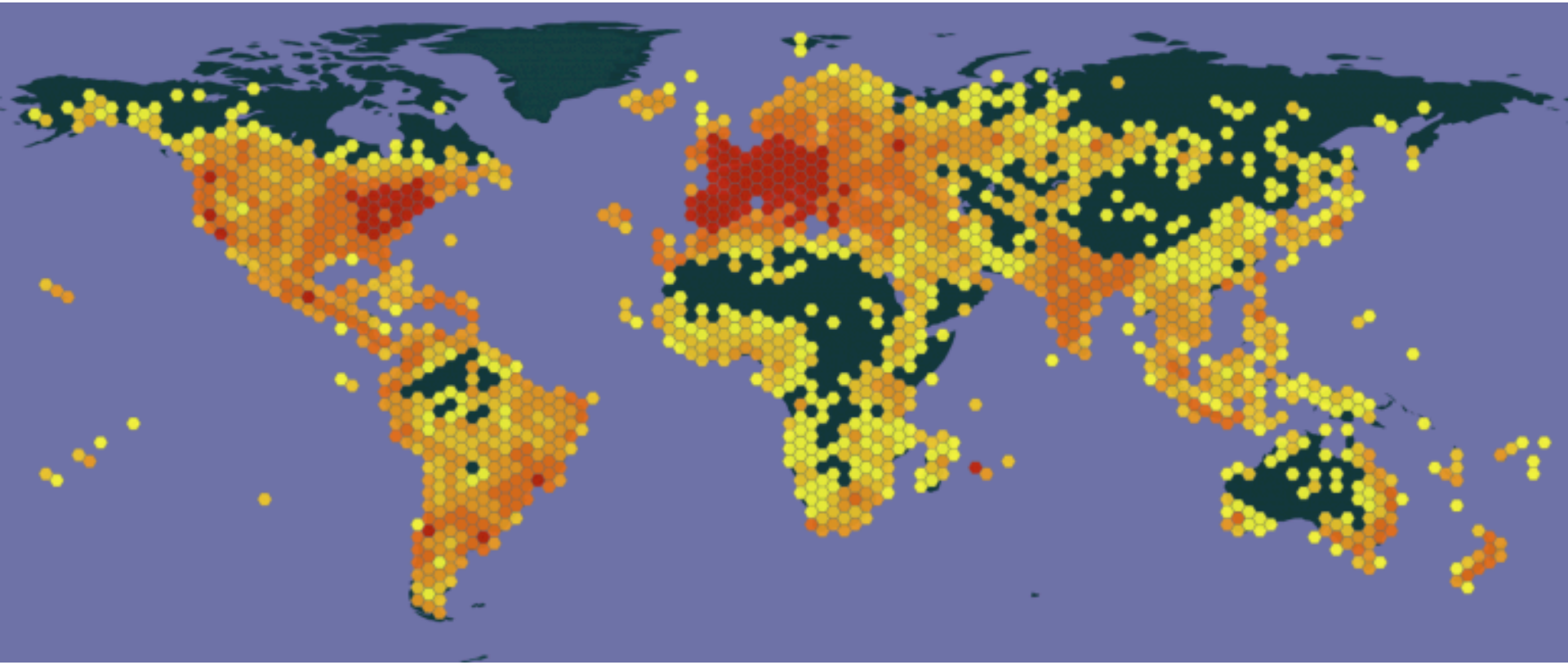
Example: Pl@ntNet



Example: Pl@ntNet

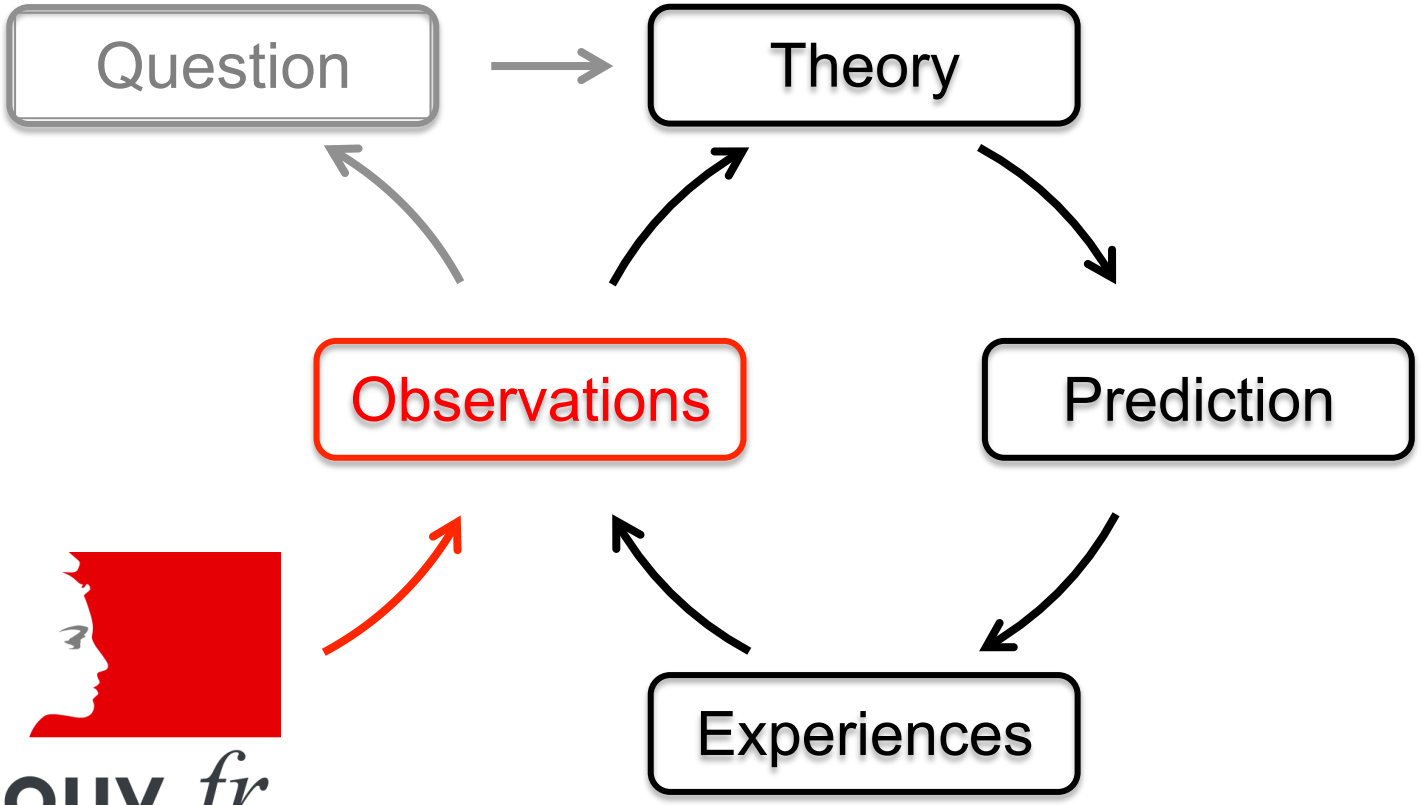
- Each Pl@ntNet user can share their data to enable global monitoring of plant biodiversity

  → GBIF (Global Diversity Information Facility)



What changed?

6. Open-data: data are public goods



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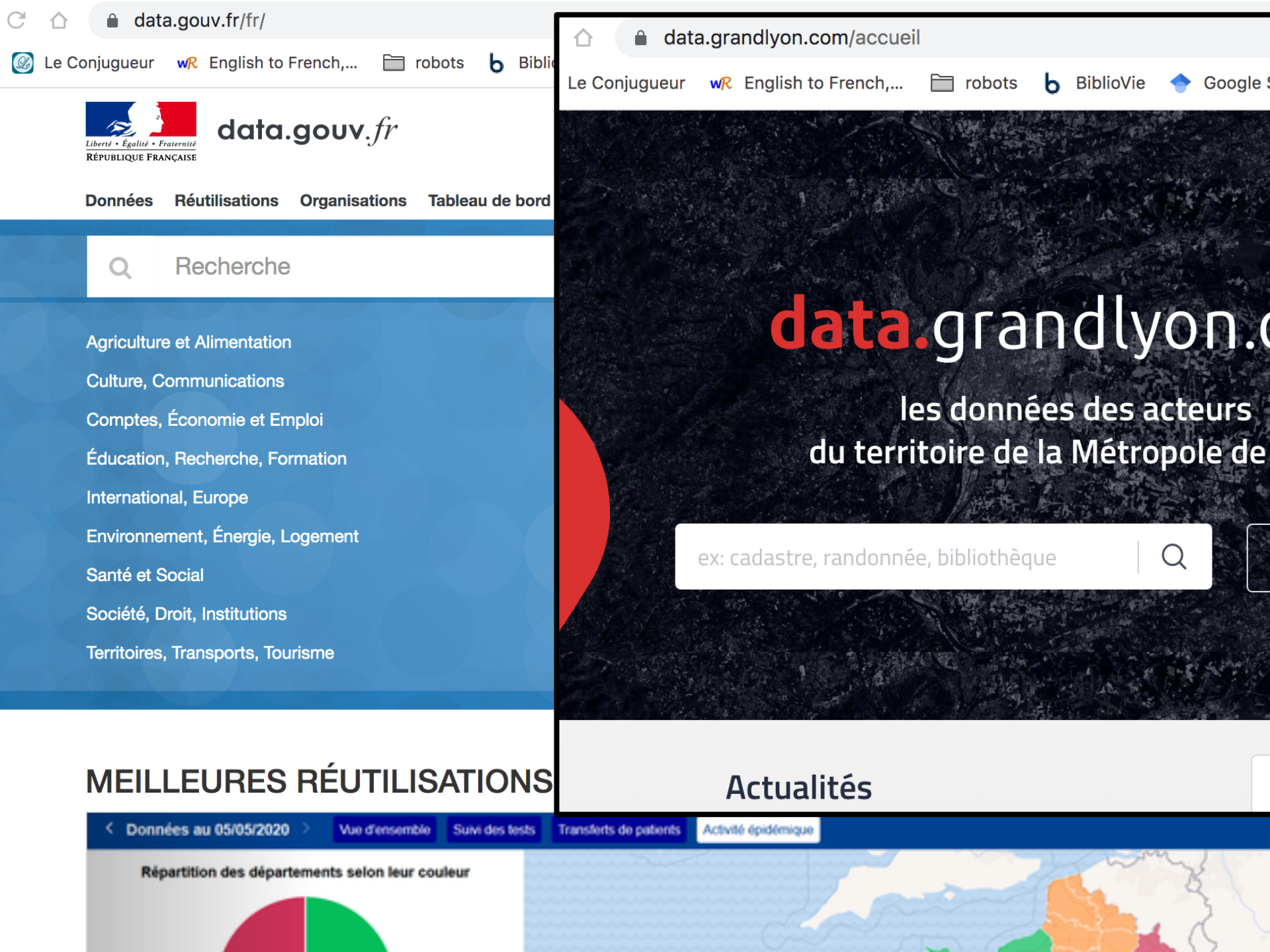
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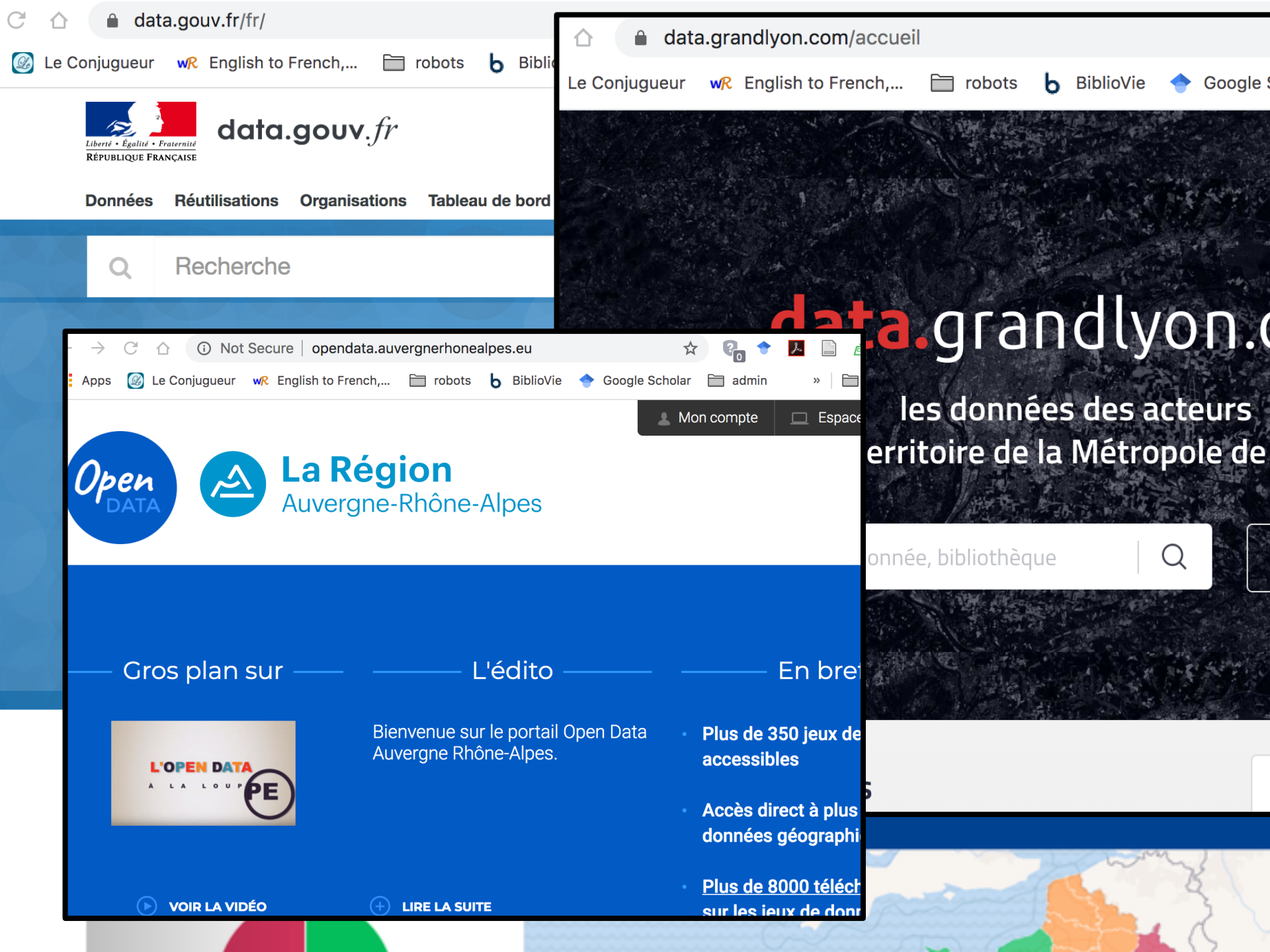
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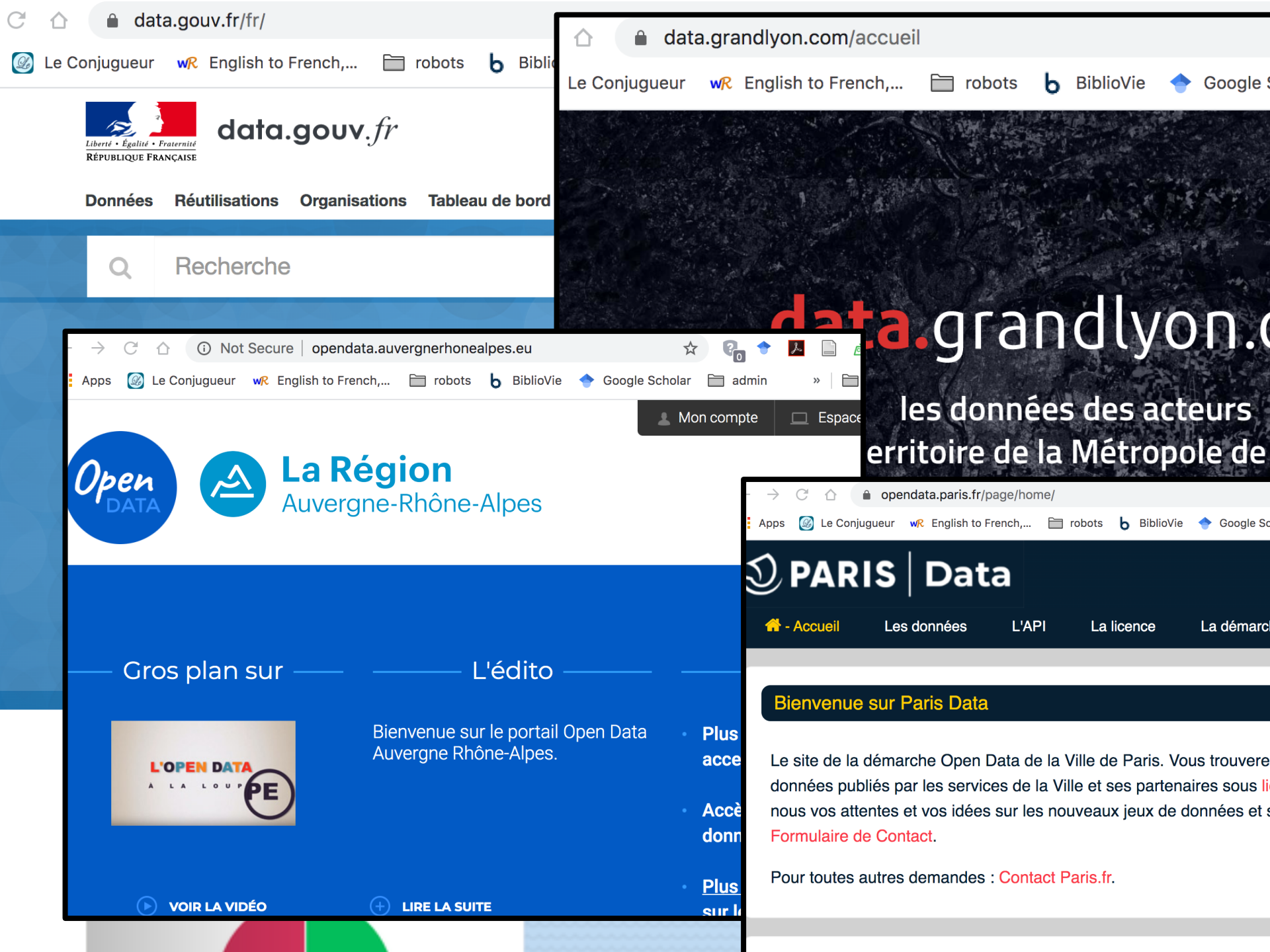
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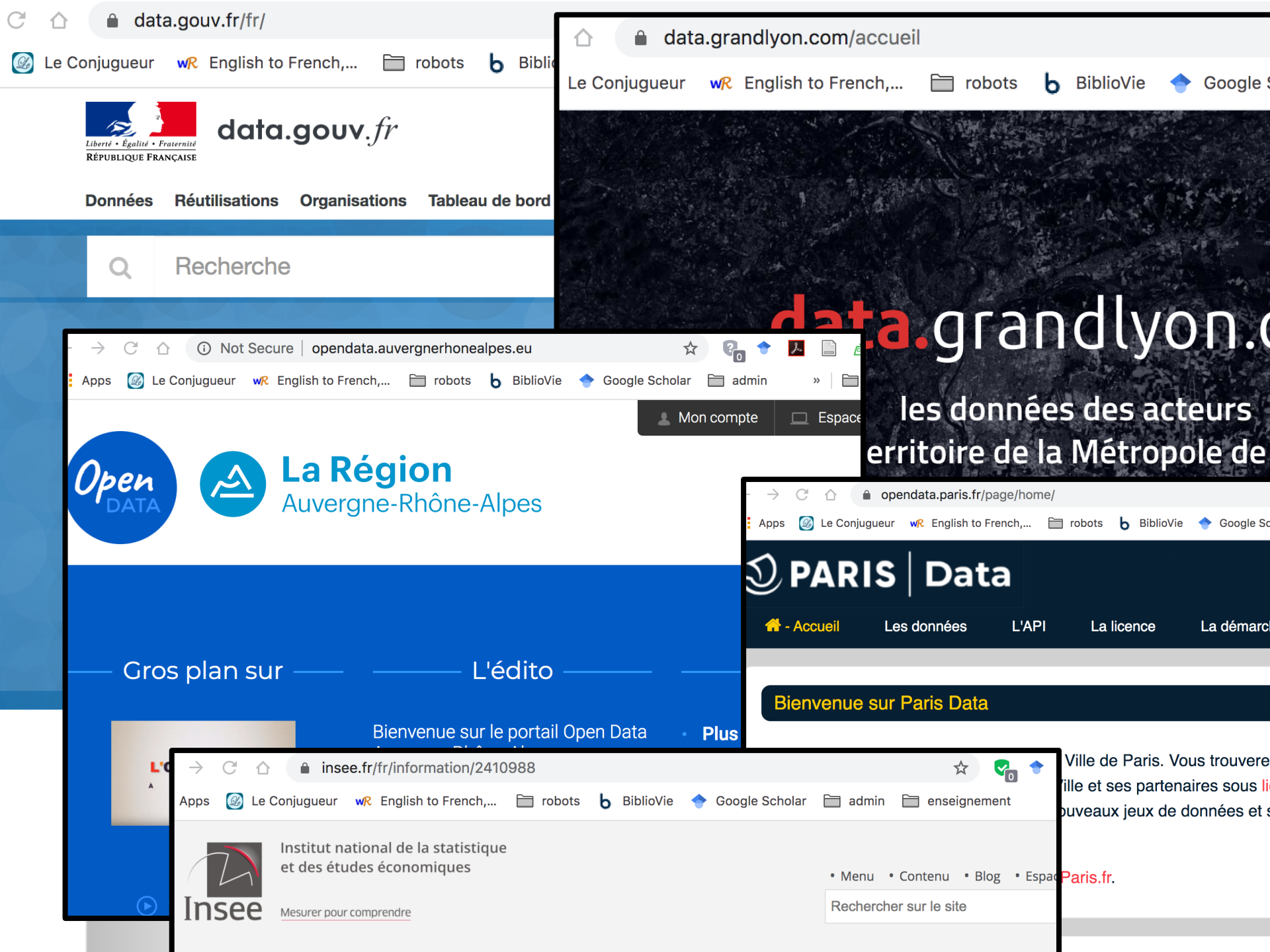
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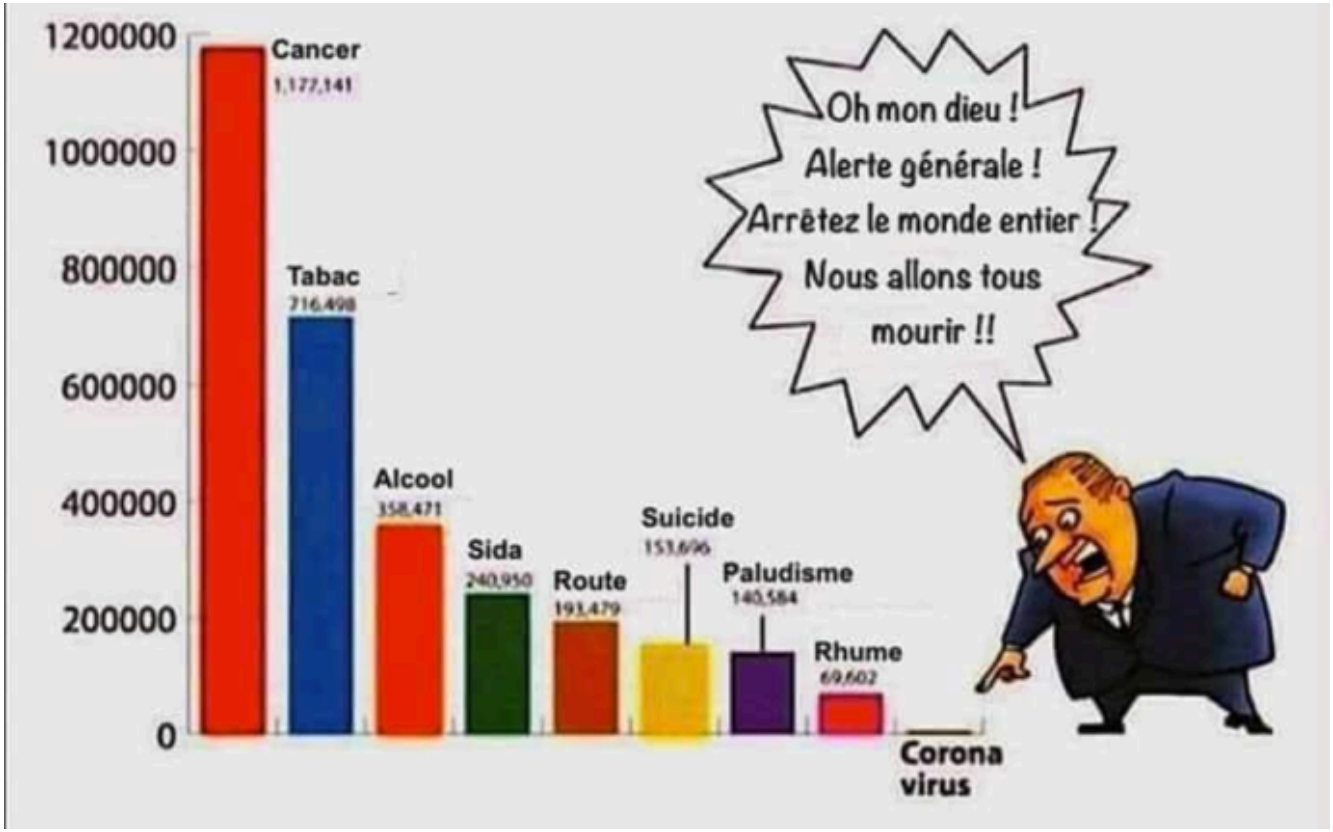
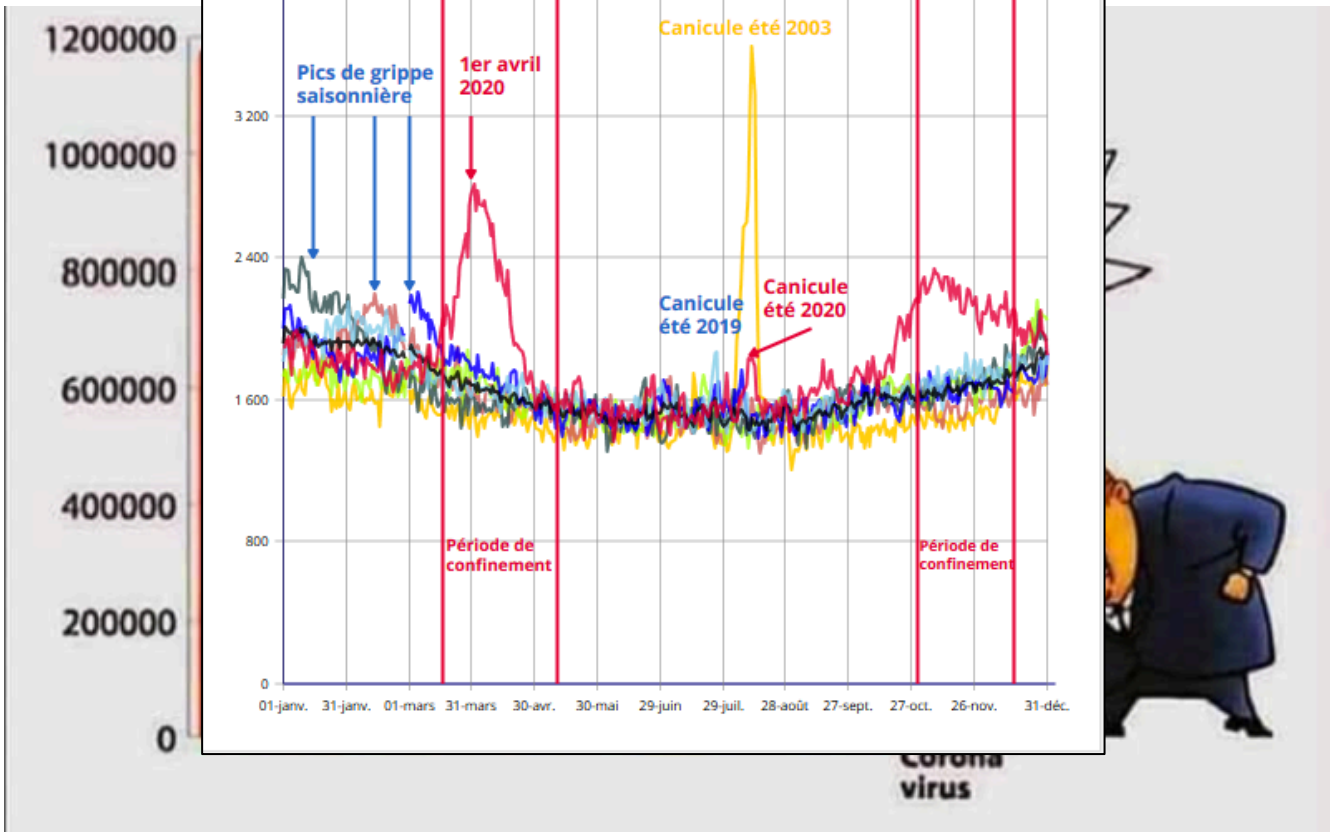
Open-Data

- Open data allows everyone to form an opinion on the "life of the city" by directly accessing factual information
  - Valorisation of data, Fact-Checking ...



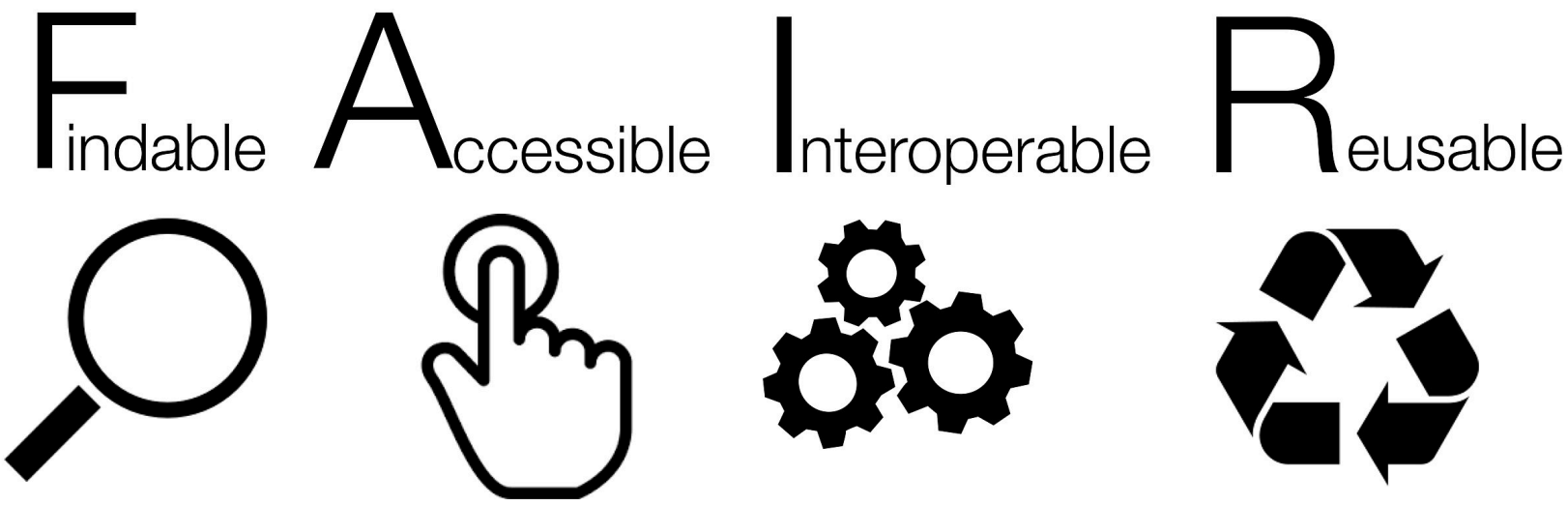
Open-Data

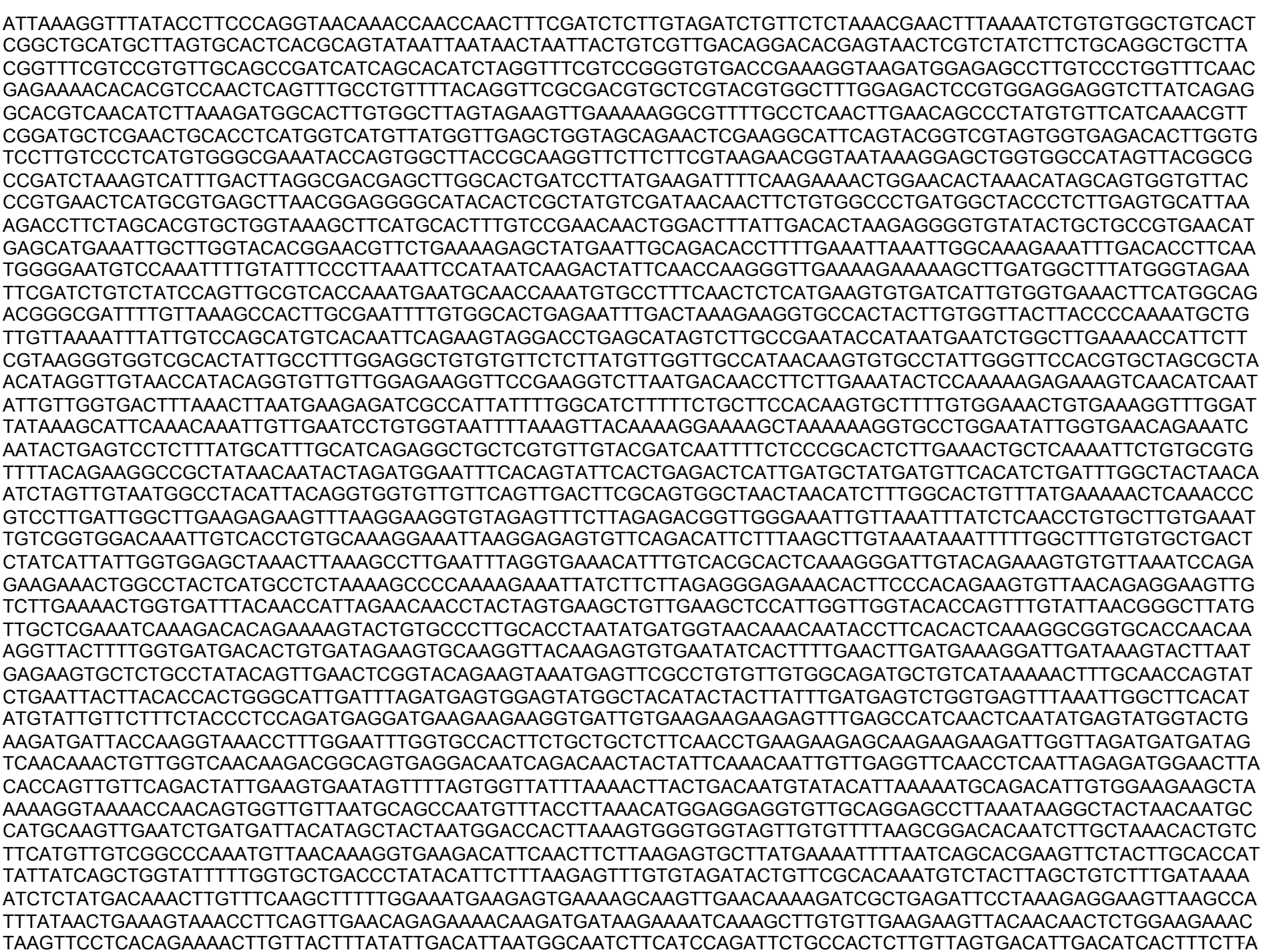
- Open data a… on the "life of the city" by … ation
  - Valorisation …



Open-Data in sciences

- Scientific data are increasingly available on the Internet (as a matter of principle and/or legal obligation)
  - Publications (Open-Access, arXiv/BioarXiv, Hal...)
  - Raw data (NCBI, Ensembl, GBIF, EMBL, JSTOR Global Plants ...)
  - Digitalisation of collections (books, herbaria, photos, ...)
- FAIR principles





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KEIDRLNEVAKNLNESLIDLQELGKYEQYIKWPWYIWLGFIAGLIAIVMVTIMLCCMTSCCS
CLKGCCSCGSCCKFDEDDSEPVLKGVKLHYT

What are the consequences of these changes?

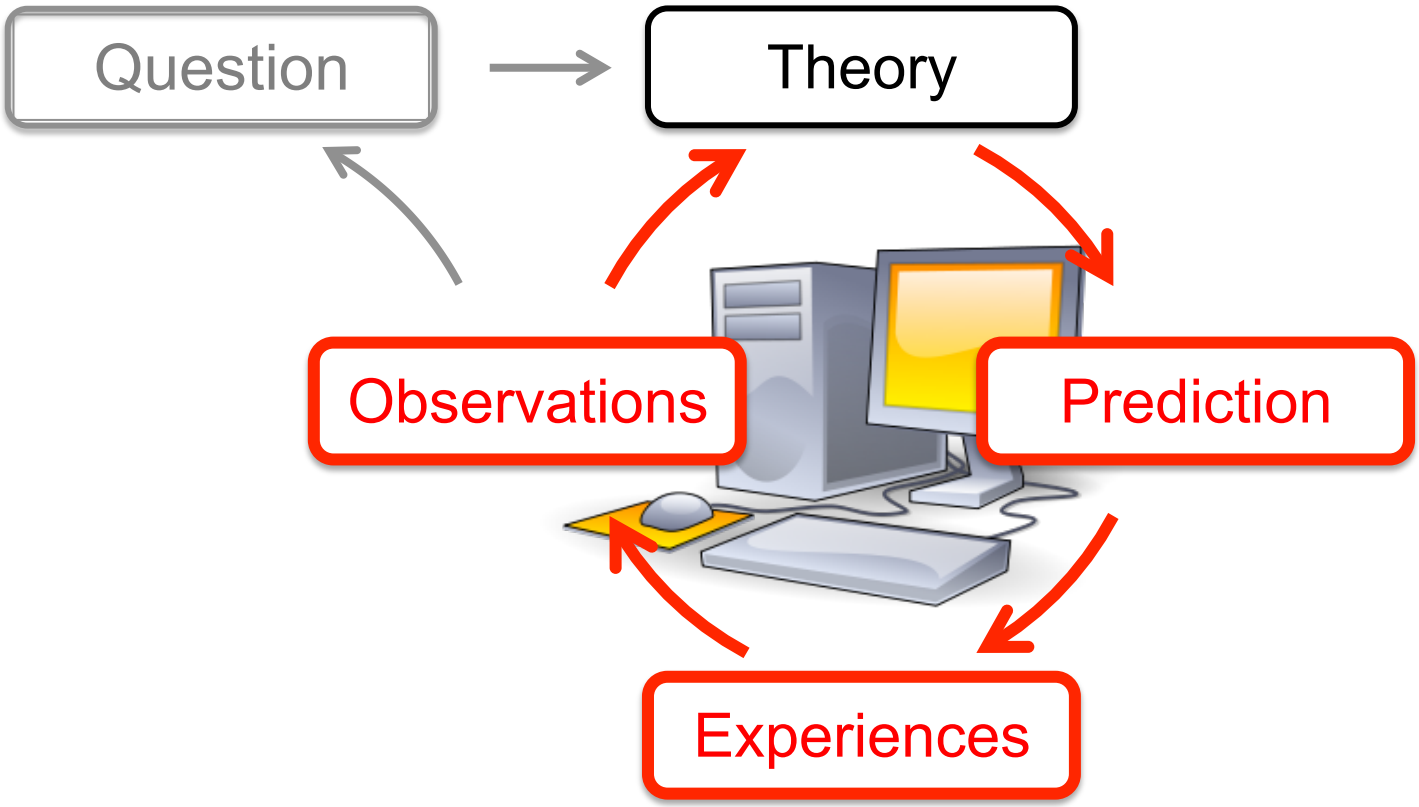
- Data available to all!
- We live in great times
- New tools, new objects, global sharing, ...

BUT

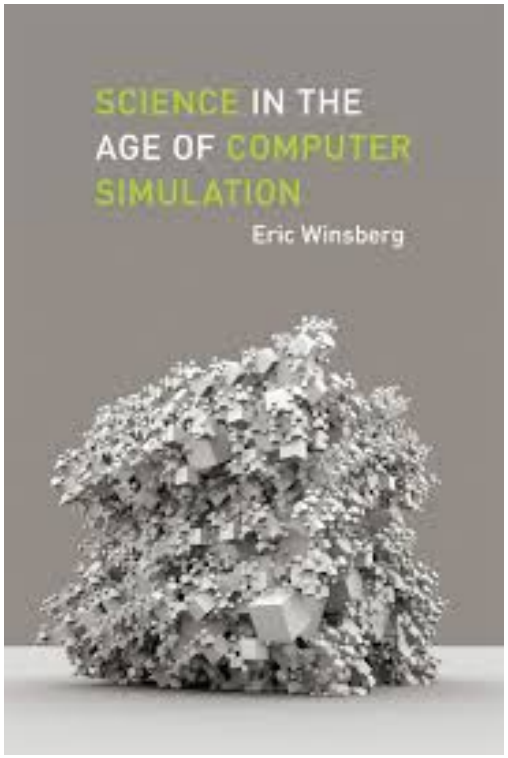
- Available does not mean accessible and usable
  - → That is the purpose of FAIR
- Accessible and usable data does not mean used data
  - → Data is only used if scientists (or the general public) are able to use it ...
  - → Science relies more and more on computer scientists
  - → Computer scientists need understanding (other) sciences!

What changed?

7. New experimental forms are being developed thanks to the power of computing machines Computational sciences



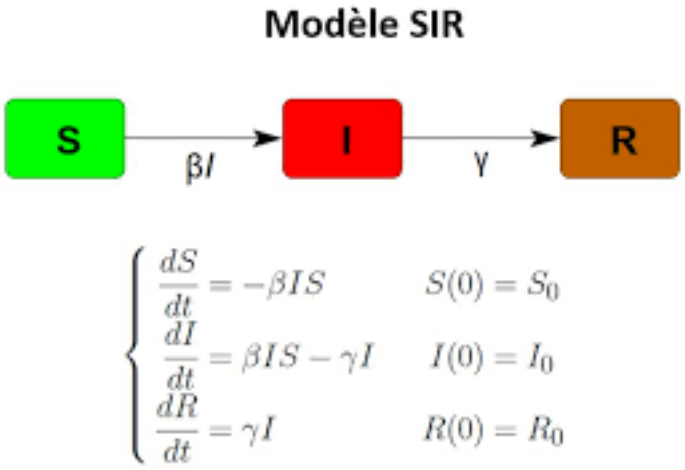
The age of computer simulations



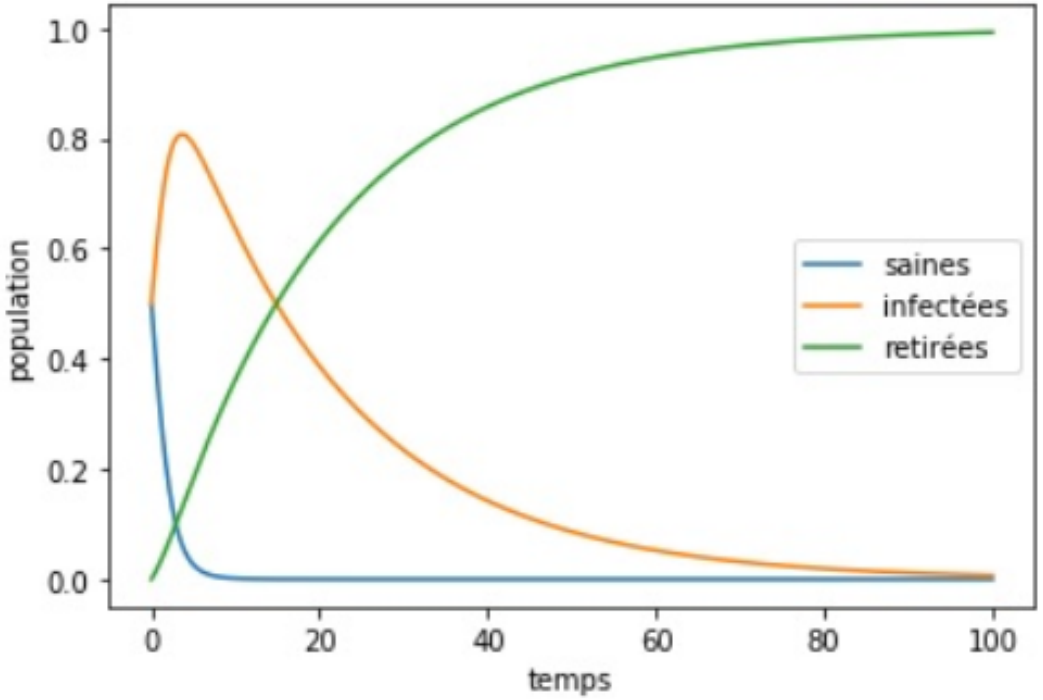
"Over the last fifty years, however, there has been a revolutionary development affecting almost all of the sciences […]. *The development I am speaking of is the astonishing growth, in almost all of the sciences, of the use of the digital computer to study phenomena of great complexity – the rise of computer simulations. More and more scientific "experiments" are, to use the vernacular of the day, being carried out "in silico"* […] *An avalanche aided in no small part by our increasing ability to use the digital computer to build tractable models of greater and greater complexity."*

(Winsberg 2010)

Example: the “SIR” model
(we will come back to this)

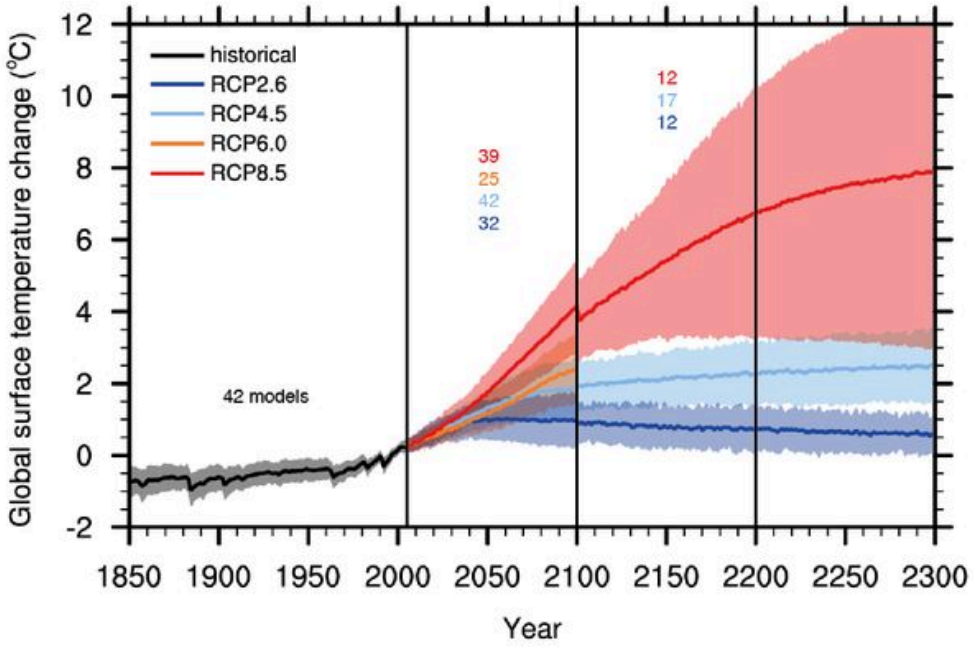


$$\begin{cases} \frac{dS}{dt} = -\beta IS & S(0) = S_0 \\ \frac{dI}{dt} = \beta IS - \gamma I & I(0) = I_0 \\ \frac{dR}{dt} = \gamma I & R(0) = R_0 \end{cases}$$



Computational sciences

- Starting from a set of theories, it is possible to use mathematical and computational tools to predict the behaviour of the system and:
- Compare to the behaviour of the real system to test the theory
- Compare to other theoretical predictions to check the internal consistency of the theories
- Replace an actual experiment when it is not practically feasible (ethically, technically or financially)
- If the model is sufficiently "safe", guide public policies, medical choices, etc.
- Example: IPCC models



At the origin of the "computational sciences

The 'PITAC' report, December 2006...

Computational Science: Ensuring America's Competitiveness

José-Marie Griffiths, Dean and Professor
School of Information and Library Science
University of North Carolina at Chapel Hill

Alan S. Inouye, PITAC Coordinator
National Coordination Office for NITRD

Chris R. Johnson, Distinguished Professor
School of Computing
University of Utah

CNI Task Force Meeting, December 6, 2005

A Report of the PITAC

President's Information Technology Advisory Committee (PITAC)

[…]

Remember!

« Un enseignement de la science qui n'apprend pas à penser n'est pas un enseignement de la science, il est un enseignement de la soumission. »

E. Schatzman,
Science et société, 1971

Computational Science Definition

Computational science is a rapidly growing multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems.

Computational science fuses three distinct elements

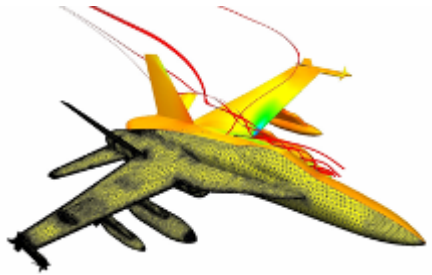
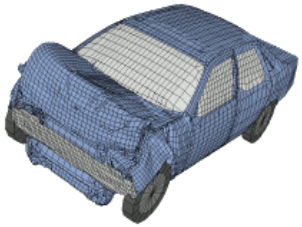
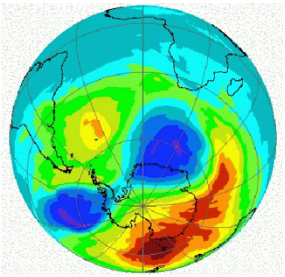
- *algorithms* (numerical and non-numerical) and *modeling and simulation software* developed to solve science (e.g., biological, physical, and social), engineering, and humanities problems;
- *computer and information science* that develops and optimizes the advanced system hardware, software, networking, and data management components needed to solve computationally demanding problems; and
- *the computing infrastructure* that supports both the science and engineering problem solving and the developmental computer and information science.

What is Computational Science? Applications

- Social sciences: Modeling in macroeconomics
- Physical sciences: Discovering brown dwarves
- National & homeland security: Modeling the spread of infectious diseases
- Geosciences: Predicting severe storms
- Engineering and manufacturing: Converting biomass to ethanol
- Biological sciences and medicine: Identifying brain disorders

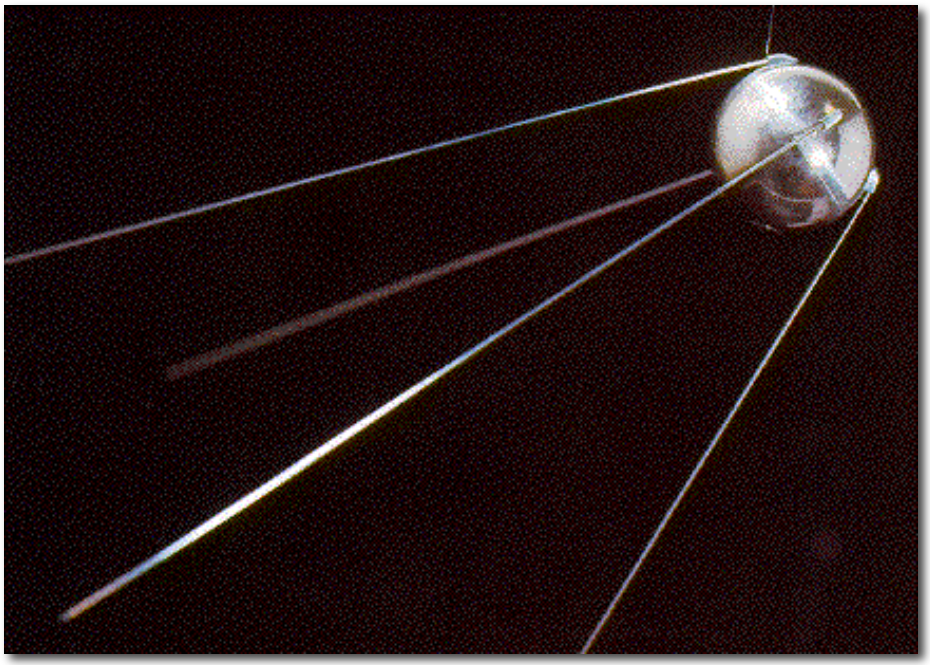
The Third Pillar of 21st Century Science

- Three pillars
  - theory, experiment, and *computational science*
- Computational science enables us to
  - investigate phenomena for which economics or constraints preclude experimentation
  - evaluate complex models and manage massive data volumes
  - model processes across interdisciplinary boundaries
  - transform business and engineering practices


A Wake-up Call:

The Challenges to U.S. Preeminence and Competitiveness

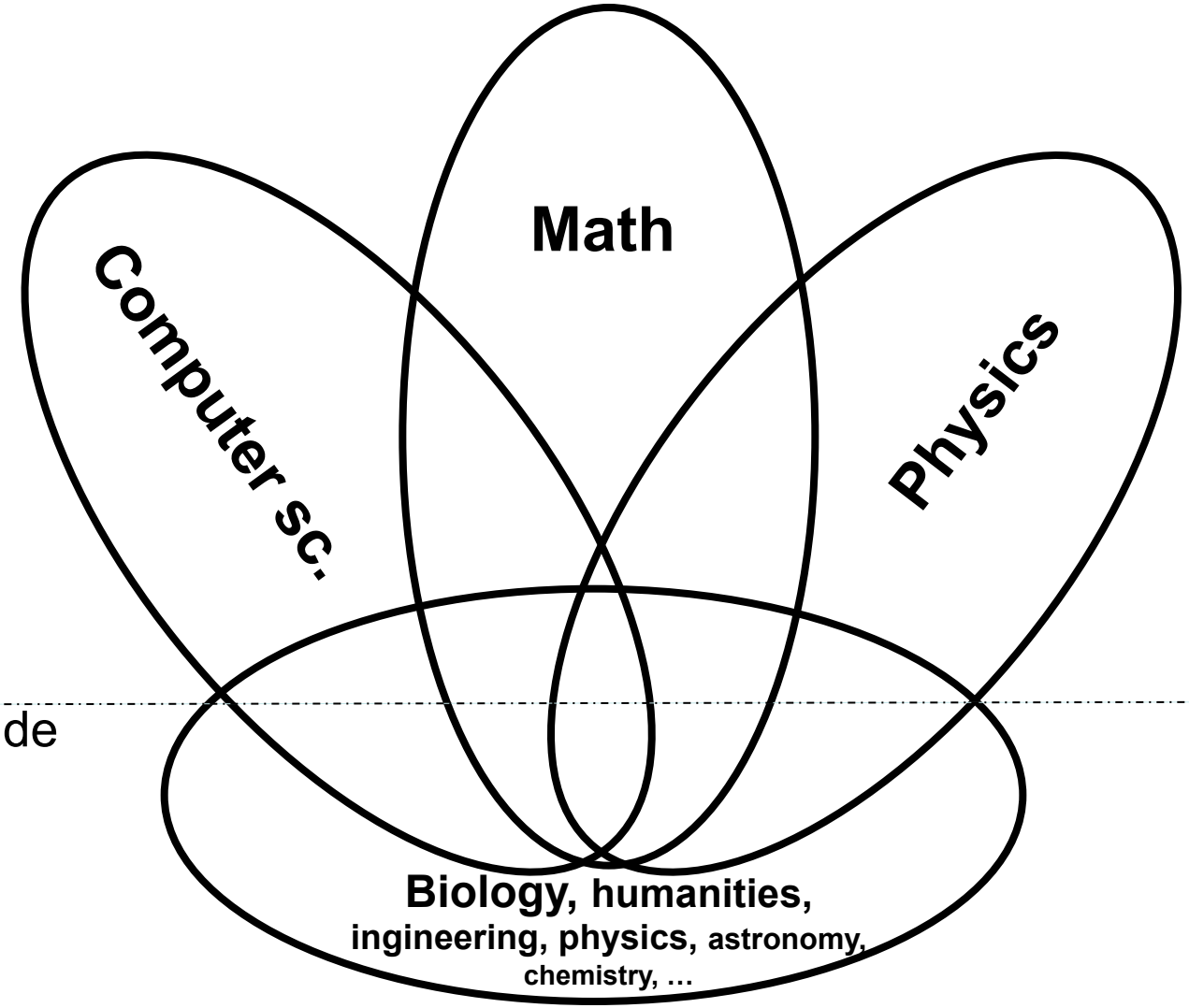


Sputnik: October 4, 1957

What are computational sciences ?

- A third pillar of science?
  - Theory, experiment... And “modelling/simulation”?
- But :
  - Computational sciences use theory and experimentation like all other sciences!
  - Virtually “all” sciences have “always” (at least since Galileo) used modelling and models (mathematics models among others)

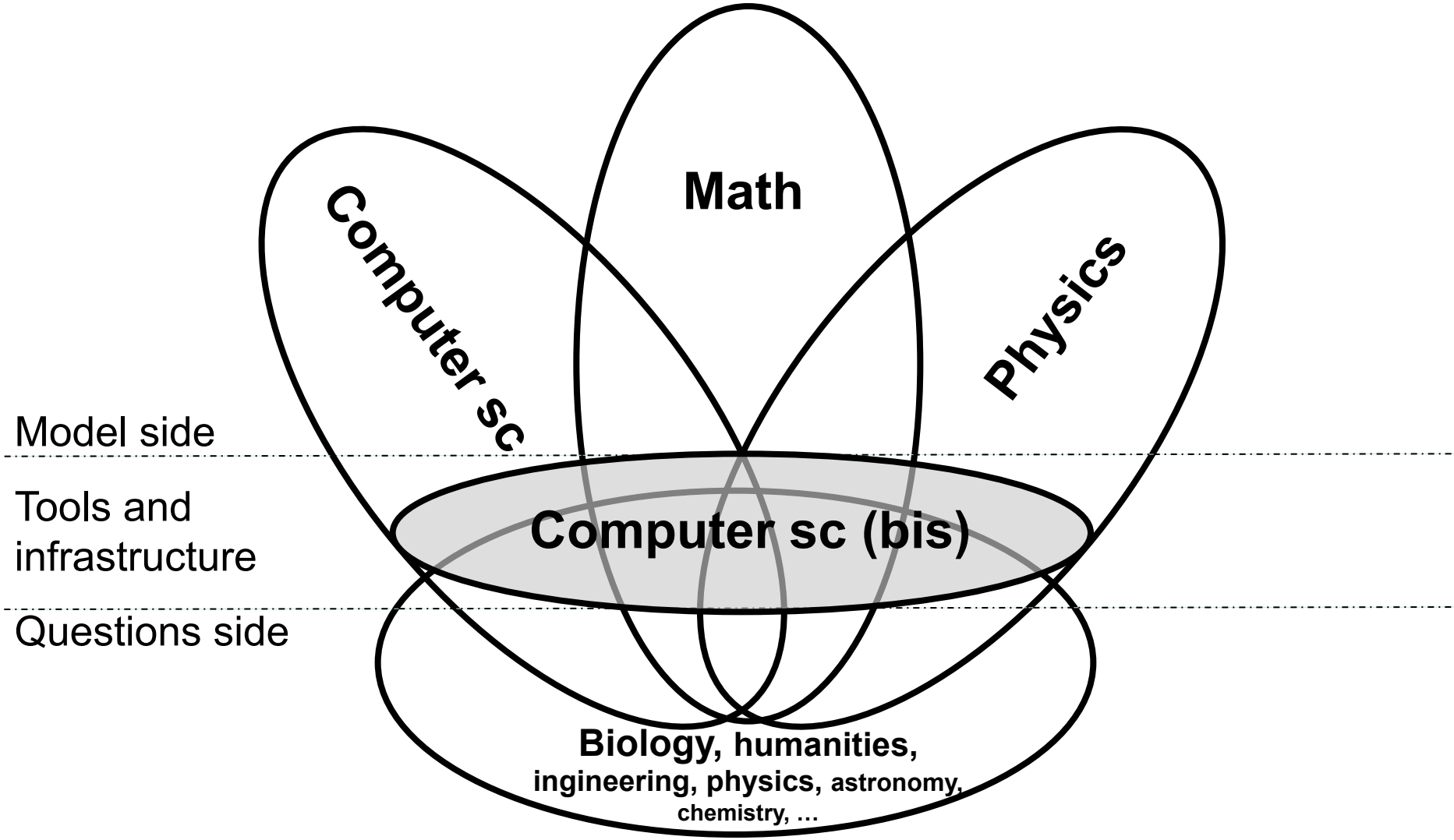
Modelling has been around “forever”



Model side

Questions side

What changed?



What are computational sciences?

- A third pillar of science?
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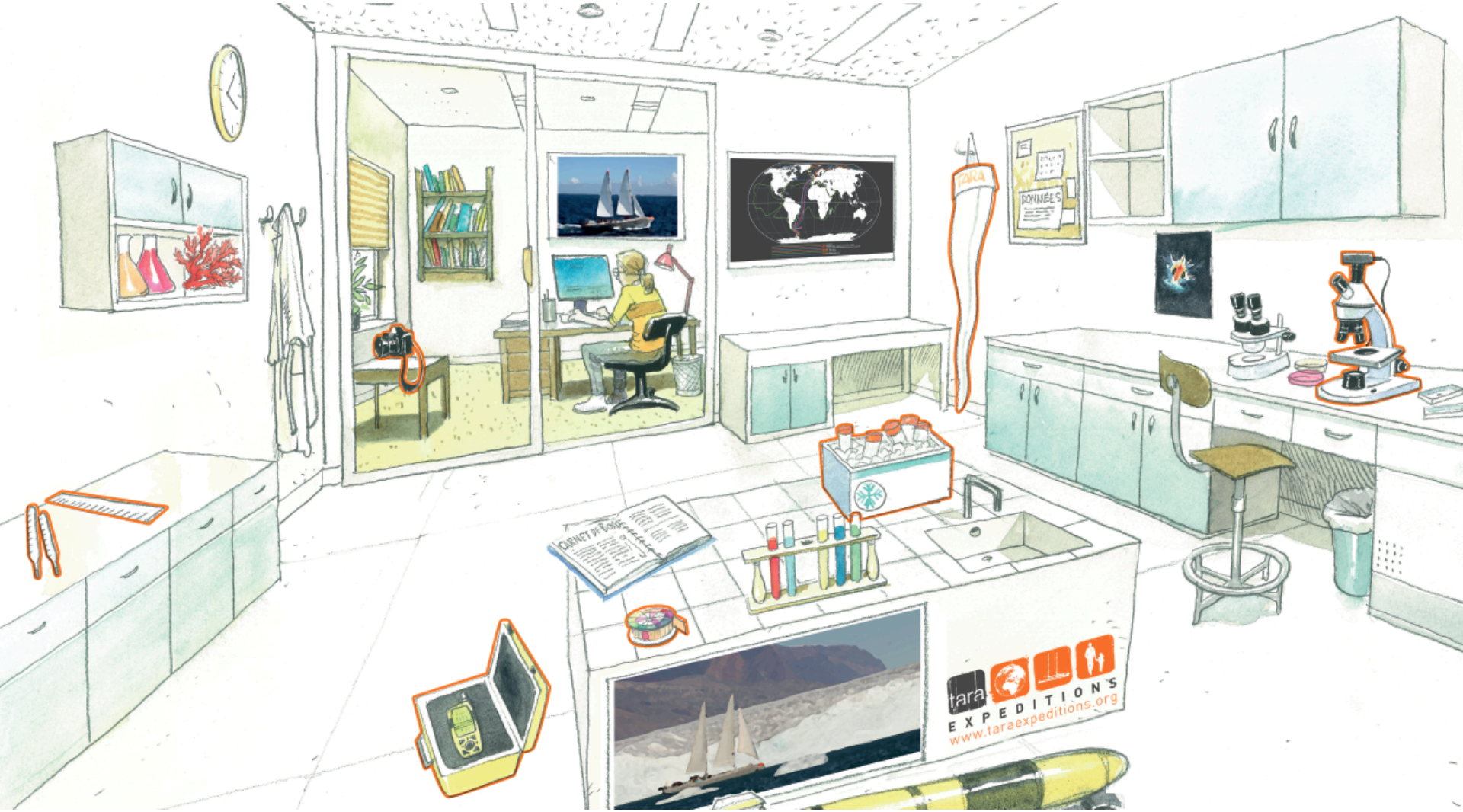
- But :
  - Computational sciences use theory and experimentation like all other sciences!
  - Virtually “all” sciences have “always” (at least since Galileo) used modelling and models (mathematics models among others)
- Computational sciences are NOT a third pillar
  - They are an extension of the first two pillars: by integrating the use of the computer as a computational tool, computational sciences increase the capabilities of models tenfold
  - They allow the study, through modelling and computer simulation, of systems to which we did not have access “before”

Research, Science an Computational Sciences

Conclusion?

Life of a life scientist...



https://oceans.taraexpeditions.org/


Je ne comprends pas. Là où vous cherchez, il n'y a ... rien ?


Oui, mais là au moins il y a de la lumière !