Computational Science and Engineering

Malik Ghallab

LAAS-CNRS

April 2013

Centuries of craftsmanship development

M. Al Khawarizmi
780 - 850

Tycho Brahe
1546 - 1601

J. Kepler
1571 - 1630

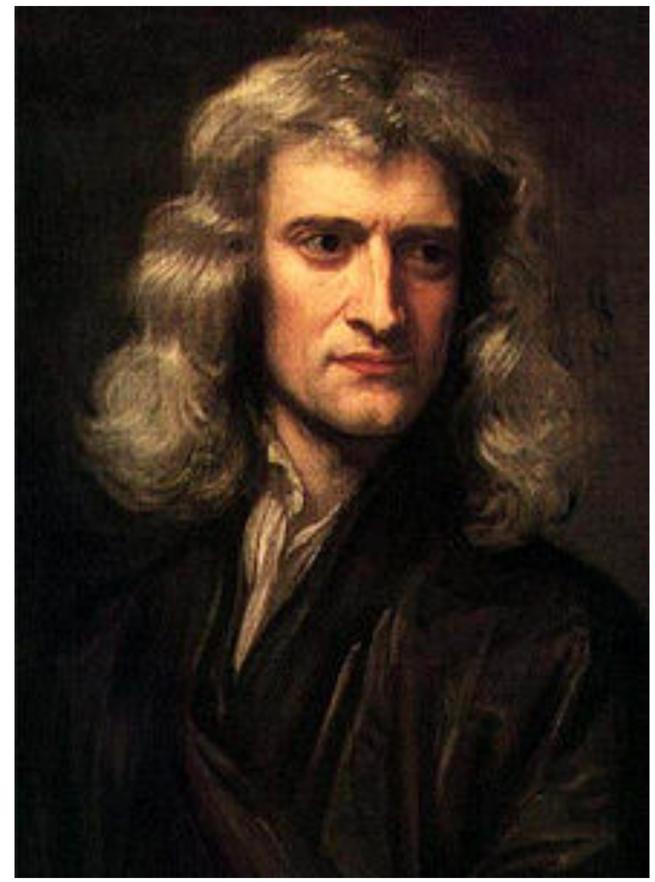
E. Hubble
1889 - 1953

S.Hawking

Centuries of craftsmanship development

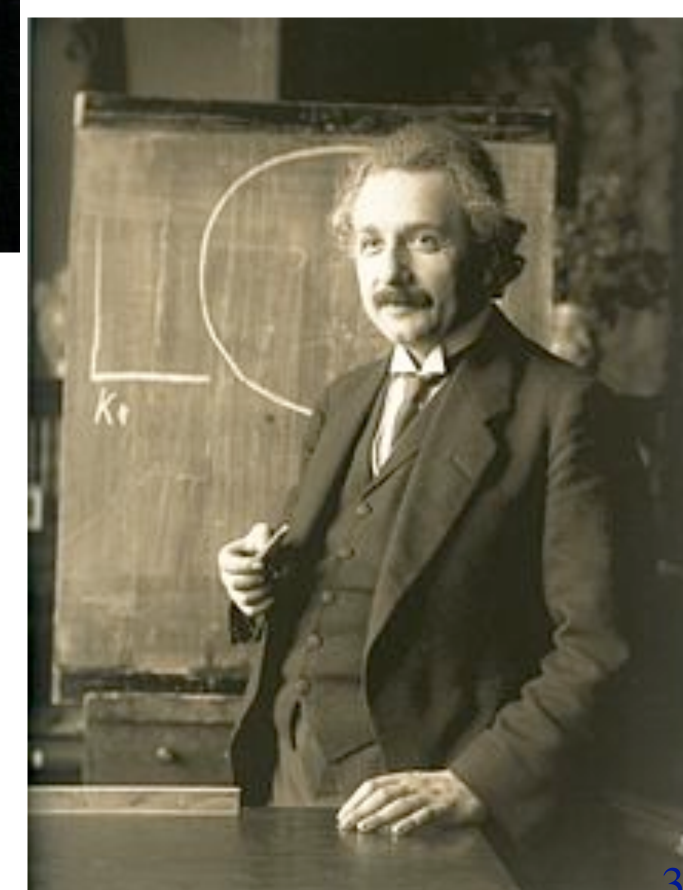
C. Ptolemy
90 - 168

G. Galileo
1564 - 1642



I. Newton
1642 - 1727

A. Einstein
1879 - 1955



Centuries of craftsmanship development

Past methods

- Data: notebooks, few Kb
- Computation: by hand, few flops
- Theory: driven by data and computation
- Team: 1 bright scientist, few students

In Gravitational Physics:
- Centuries of small science, small data culture
- Few decades of radical change

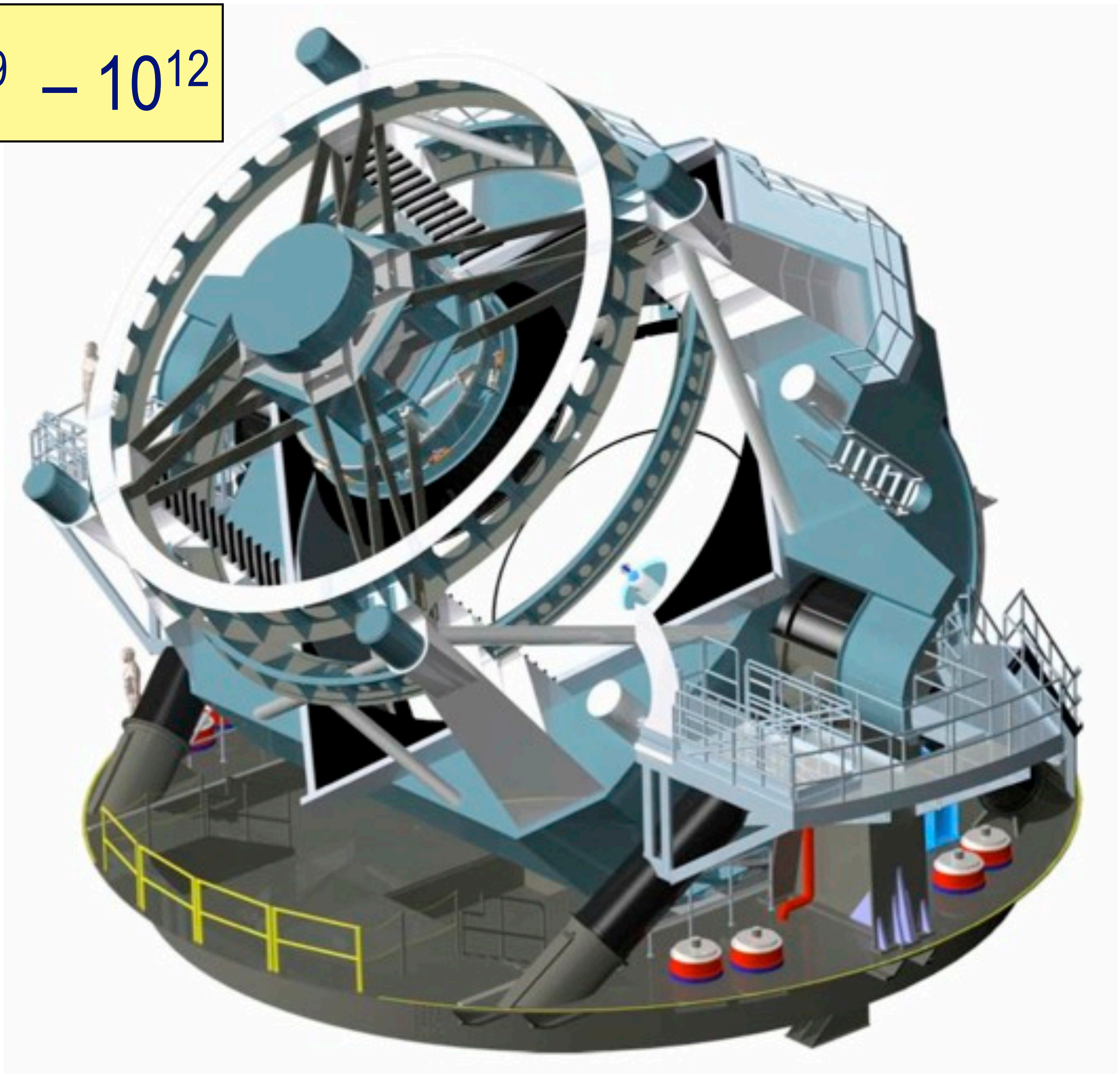
[E. Seidel, NSF]

Few decades of radical change

Unprecedented growth in

- Computation
- Data handling
- Communication
- Sensing

$10^9 - 10^{12}$



Large Synoptic Survey Telescope: 40 TBytes/night

Few decades of radical change

Allow science and engineering to address complex challenges

- Involving
  - Numerous ***coupled*** phenomena
  - Widely dissimilar entities and interactions
- Requiring very fine views of ***microscopes*** and ***telescopes*** as well as global *integrative* views of "***macroscopes***"
- Supporting difficult decisions

We seek solutions.
We don't seek – dare I say this ? – just scientific papers anymore.

[S. Chu, DoE]

Outline

- ✓ Motivations
- Ingredients of Computational Science & Engineering
  1. Modeling, simulation and computing
  2. Instrumentation, sensing and imaging
  3. Massive data processing
- Impacts of Computational Science & Engineering
- Conclusion

Ingredients of Computational Science & Engineering

New engines of science and technology

1. **Computational modeling, simulation and computing**

2. **Instrumentation, sensing and imaging**

3. **Massive data processing, mining, analyzing, learning and visualizing**

Converging conceptual and practical set of tools

1. Modeling, Simulation, Computing

Methodology

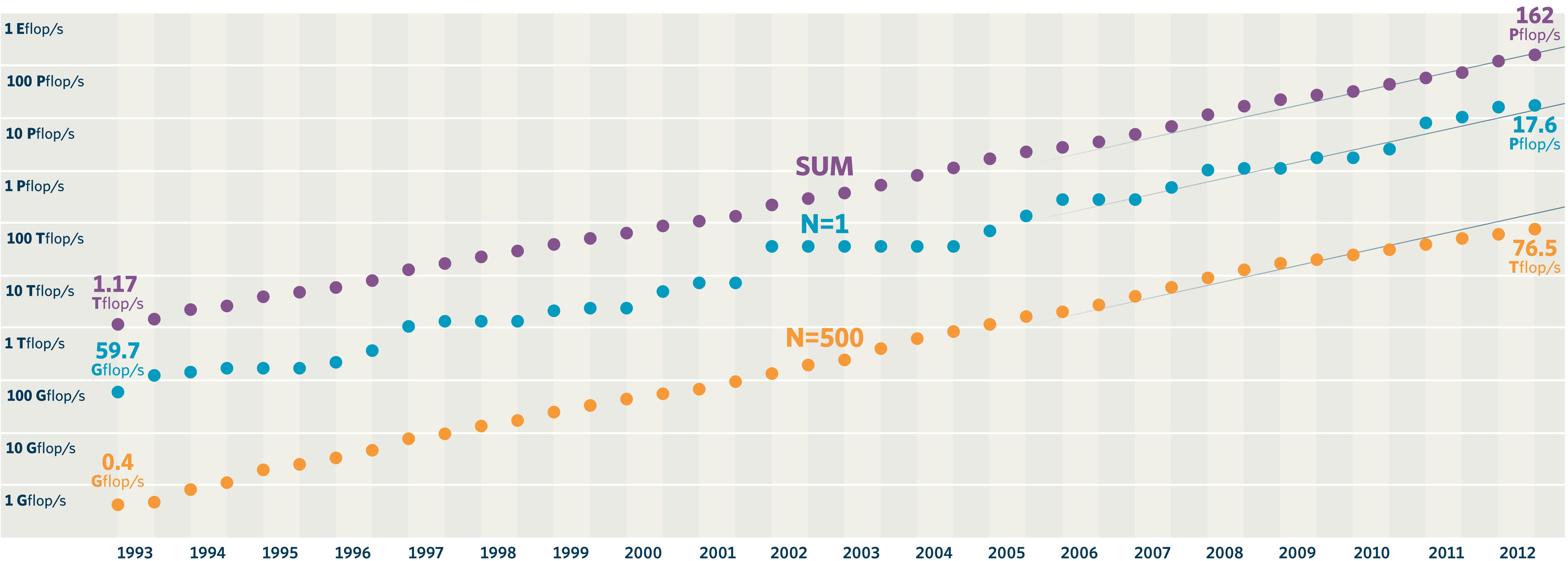
- Building computational models of a system or a phenomenon
- Analyzing properties of models
- Contrasting models to reality: identification, estimation, learning
- Designing algorithms and computational schema, parallelization, distribution
- Simulation scenarios
- Control, optimization

What's new ?

1. Modeling, Simulation, Computation

What's new ?

a) **Scaling-up** : from 10^3 flops to 10^{15} flops



[Top 500 Project]

1. Modeling, Simulation, Computation

What's new ?

a) Scaling-up : from 10^3 flops to 10^{15} flops

b) **Integration** of multiple heterogeneous models

- Complex problems involve the interaction of several phenomena
- Each phenomenon has to be addressed not in isolation but coupled with all relevant interacting effects

➡ ***Integration of heterogeneous mathematical formalisms***: differential, geometric, deterministic, stochastic, combinatorial into algorithms and software components

➡ ***Composition of elementary components*** to buildup increasingly more complex and encompassing models

Metaphor

[D.Sticker, DFKI]

Metaphor

[D.Sticker, DFKI]

Environment modeling

[D.Sticker, DFKI]

1. Modeling, Simulation, Computation

What's new ?

a) **Scaling-up** : from 10^3 flops to 10^{15} flops

b) **Integration** of multiple heterogeneous models

c) Universal scope

The book of the universe is written in mathematics.

[Galileo, *Il Saggiatore*, 1623]

The Galileo vision applied to an exception: only the inanimate world could be written in mathematics. This exception does not hold anymore. But the Galileo model has changed.
Nature is written in ***algorithmic language***.

[M.Serres, *Hominescence*, 2001]

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2. Instrumentation, Sensing, Imaging

Methodology

- Sense, acquire, measure
  ground facts and evidence to support science
- Over broad spectrum of scales
- Over broad spectrum of phenomena and units

What's new ?

2. Instrumentation, Sensing, Imaging

What's new ?

- Scale-up
- Integration
- Scope

+

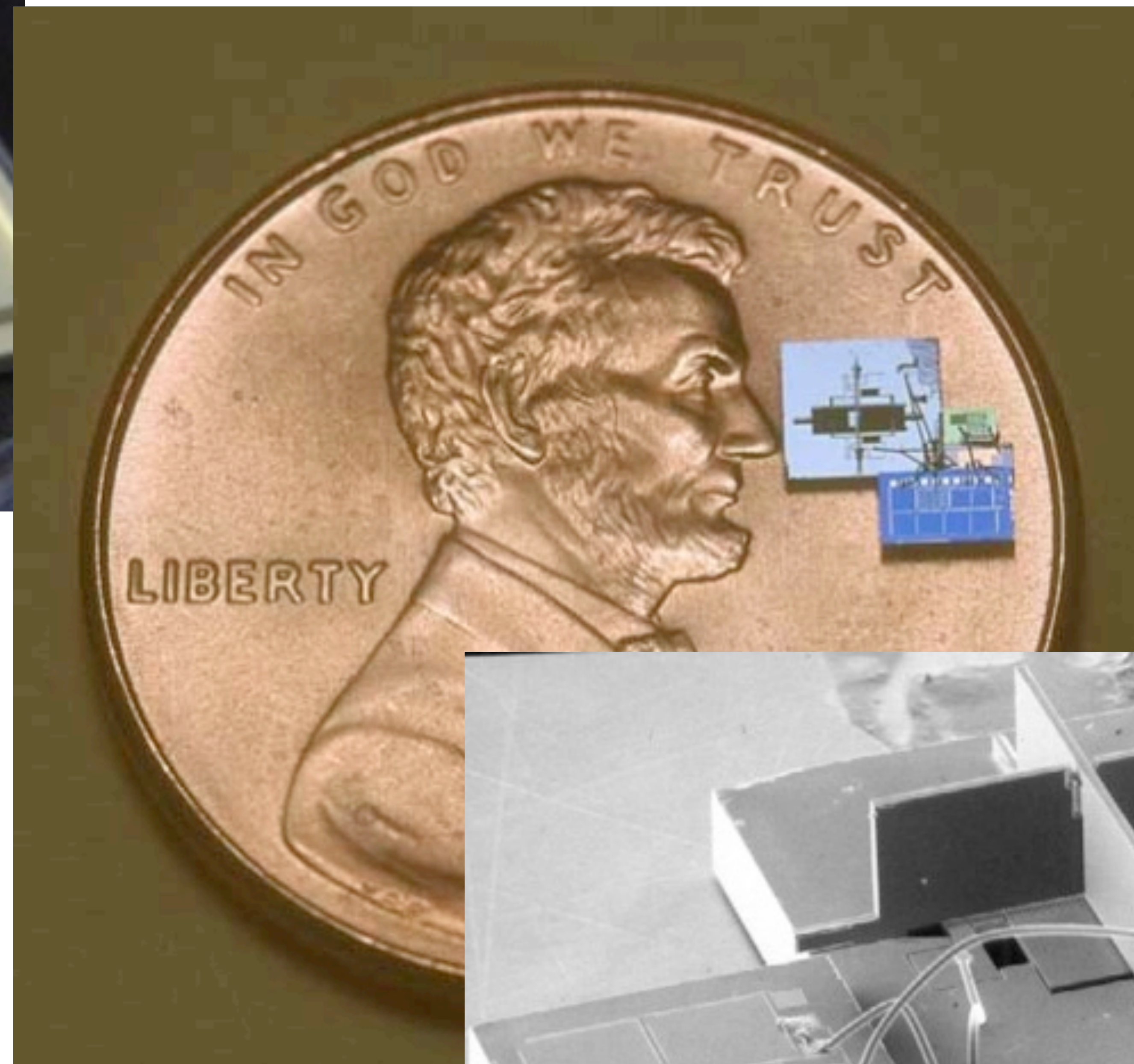
a) **Low-cost massive production**

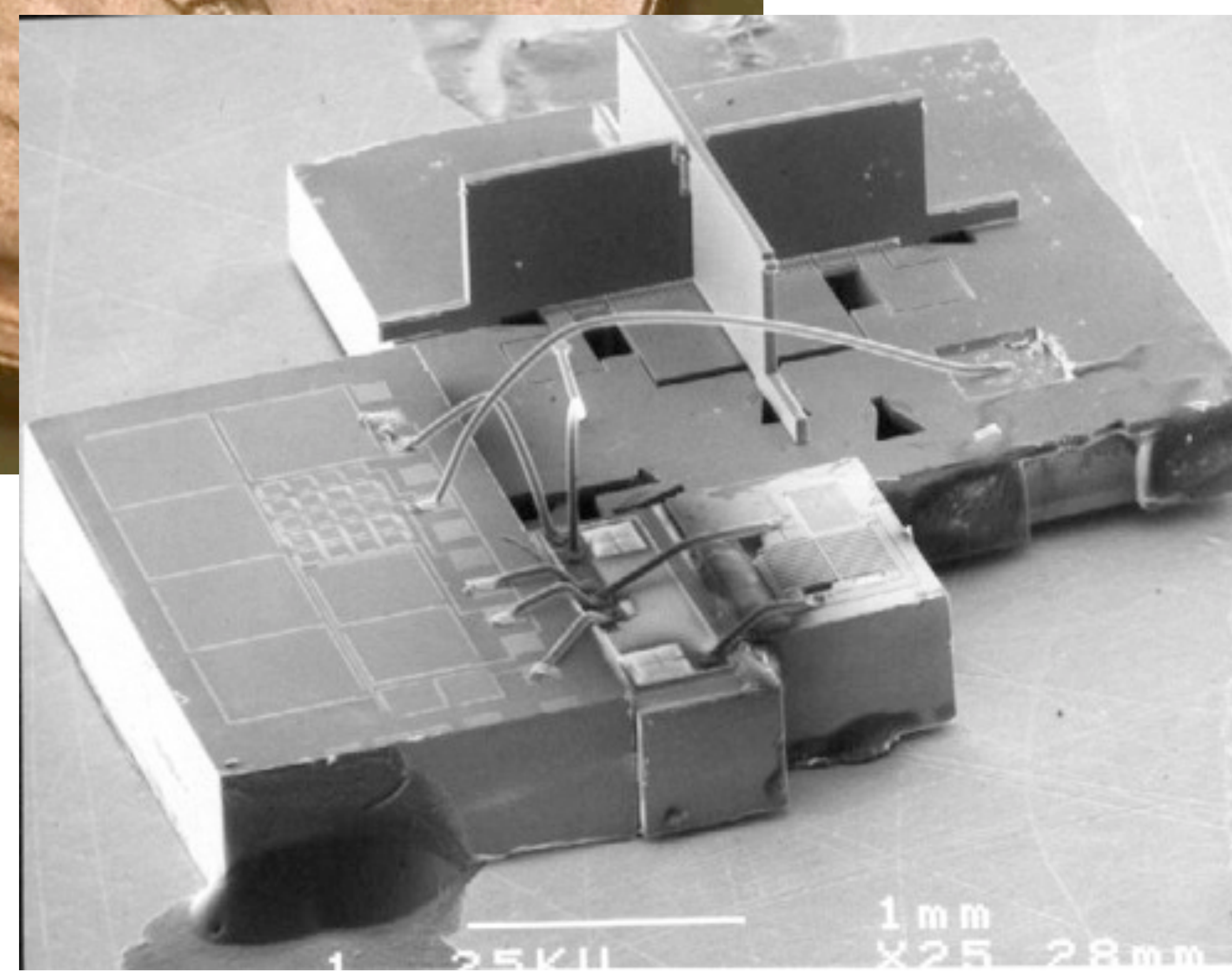
b) **Signal processing and intelligent sensor fusion techniques**

c) **Distributed, mobile and widely flexible sensors**

d) **Communicating sensors**

2. Instrumentation, Sensing, Imaging

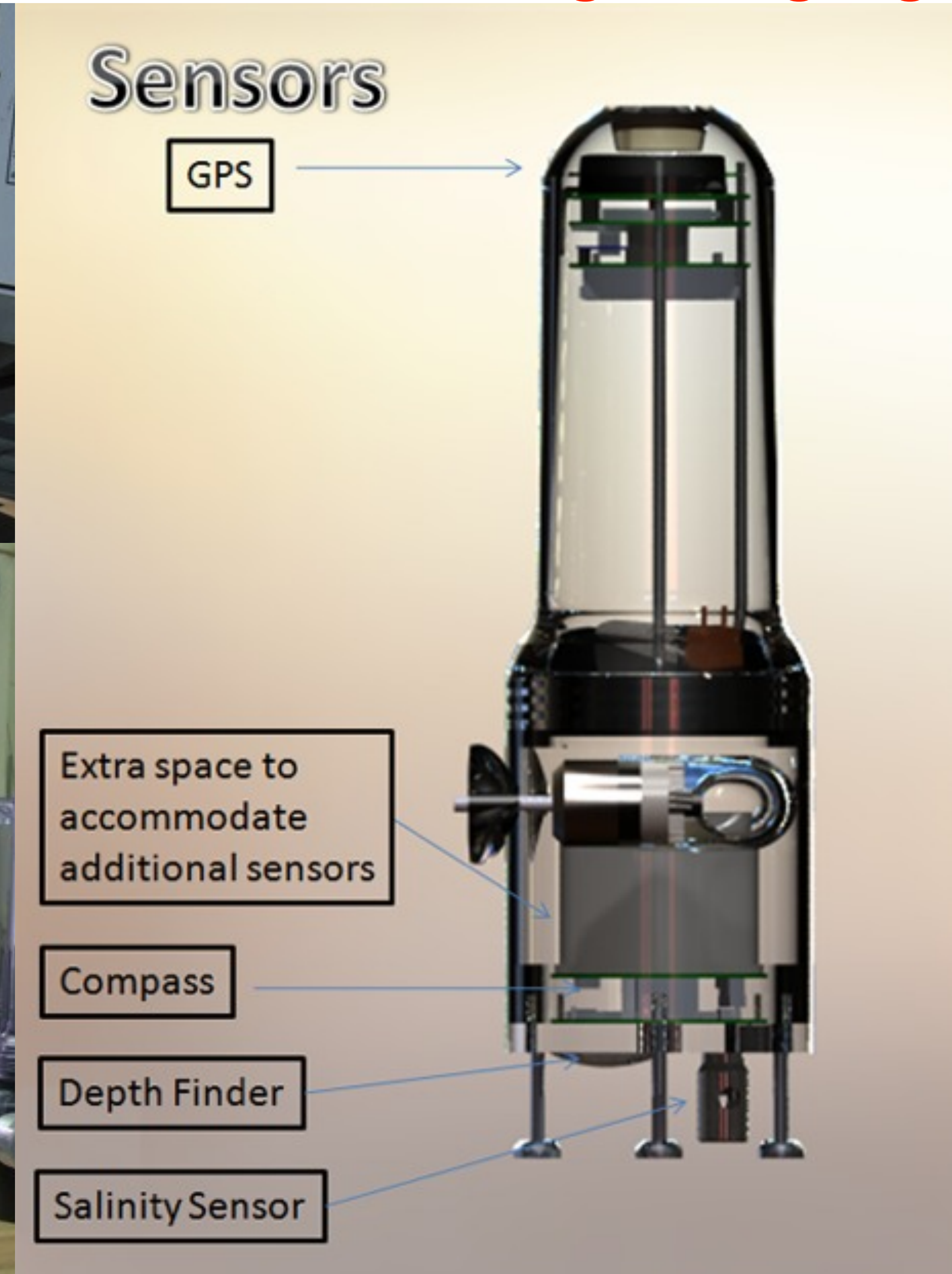




Smart dust

[K. Pister, Berkeley]

2. Instrumentation, Sensing, Imaging



Floating sensor network

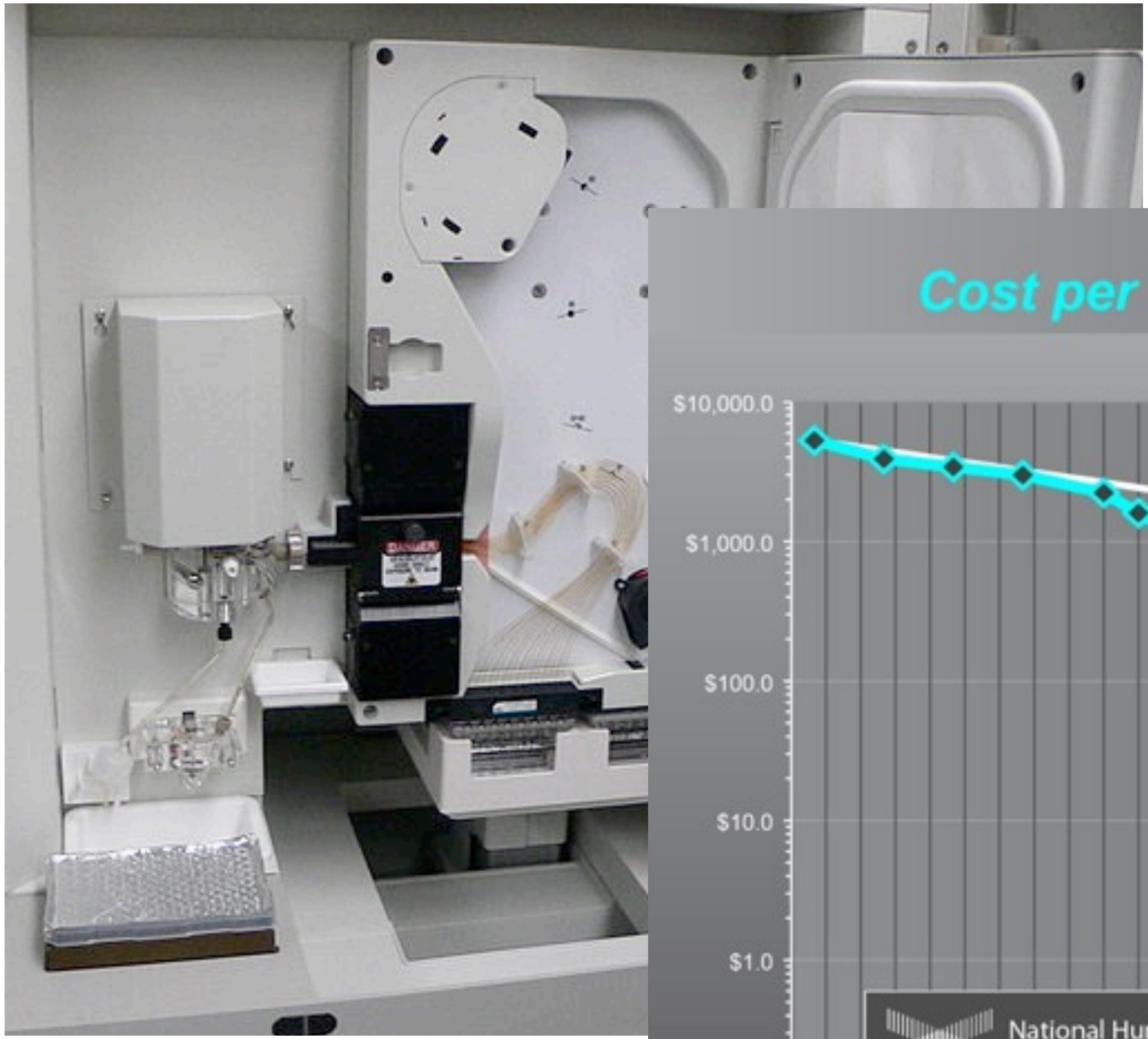
[A. Bayen, Berkeley]

2. Instrumentation, Sensing, Imaging

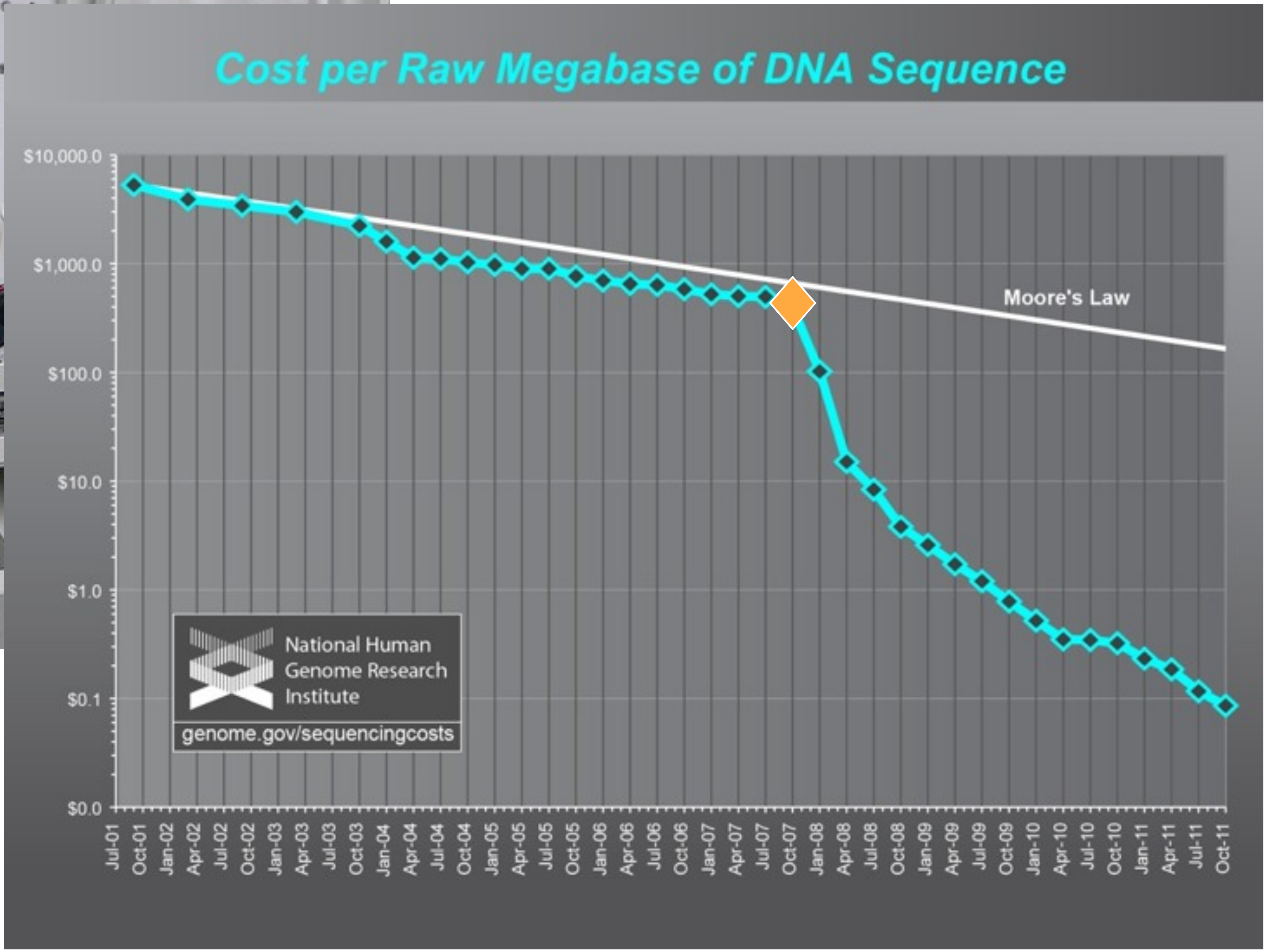
Cell scope

[D. Fletcher, Berkeley]

Instrumentation, Sensing, Imaging



DNA sequencing



[NHGRI]

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3. Massive Data Processing

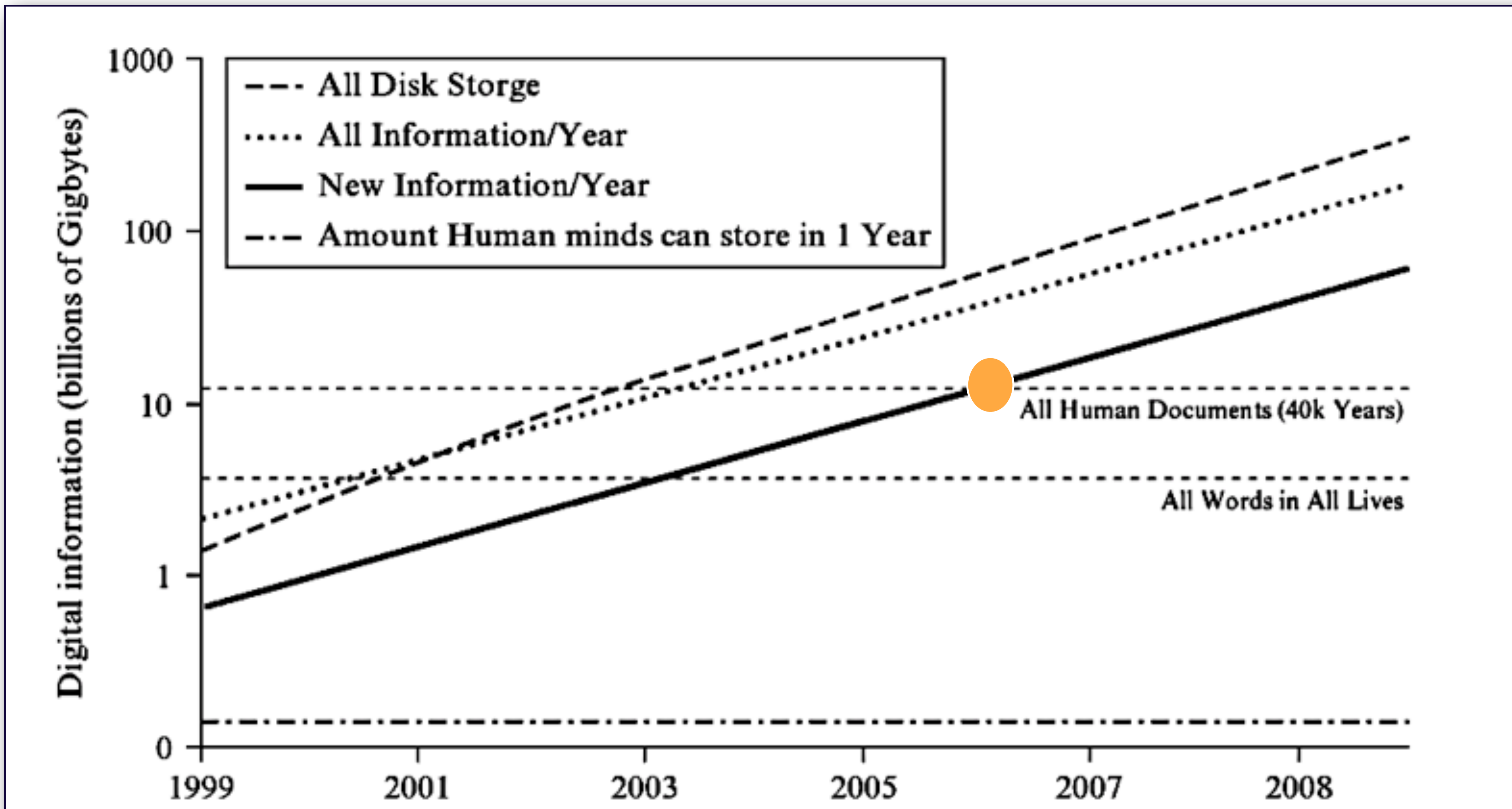
Methodology

- Collect, organize, curate
- Compare, associate, cluster into categories
- Visualize
- Correlate, associate into relations
- Interpret, generalize into knowledge

What's new ?

What's new ?

a) **Scaling-up** : from 10^3 Bytes to 10^{18} Bytes



[Lesks, Berkeley SIMS, Landauer EMC]

3. Massive Data Processing

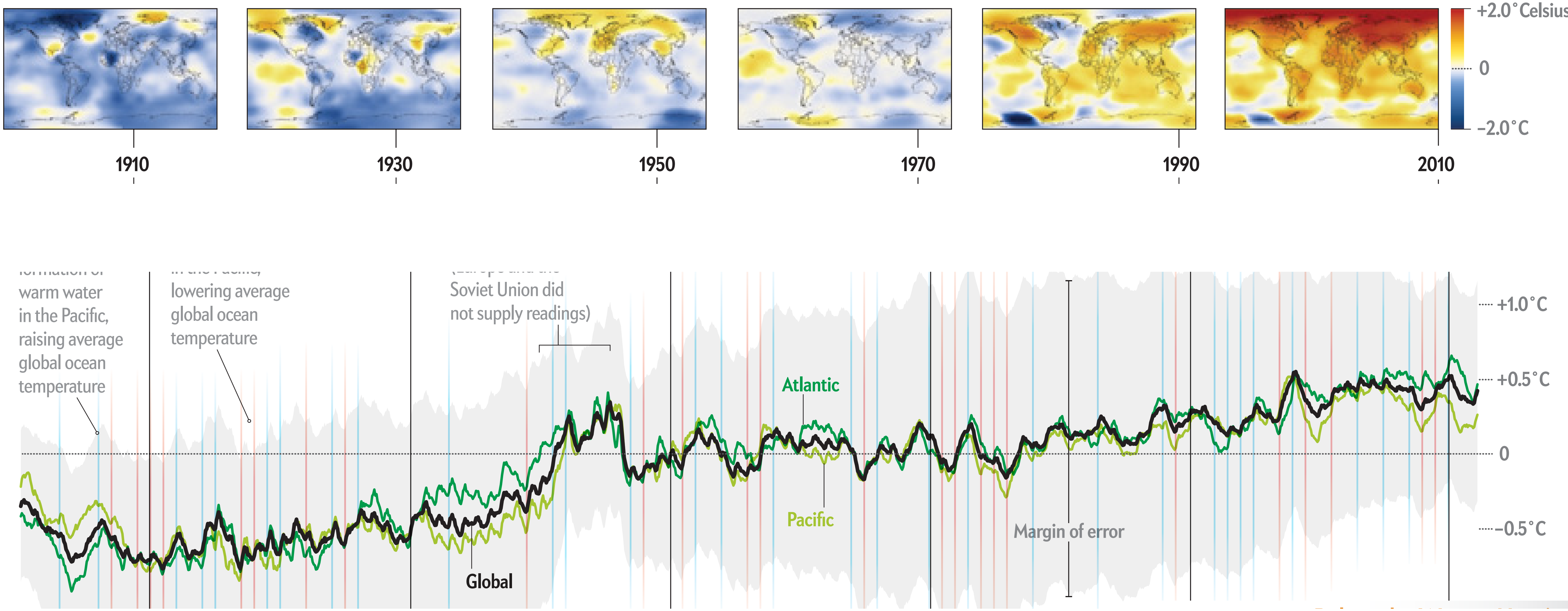
What's new ?

a) **Scaling-up** : from 10^3 flops to 10^{15} flops

b) **Integration** of data

- From sensors
- From simulations
- From broad ranges of phenomena
- Over wide space and extended time

Ocean Temperature Rise



[Scientific American, April 2013]

3. Massive Data Processing

What's new ?

a) **Scaling-up** : from 10^3 flops to 10^{15} flops

b) **Integration** of data

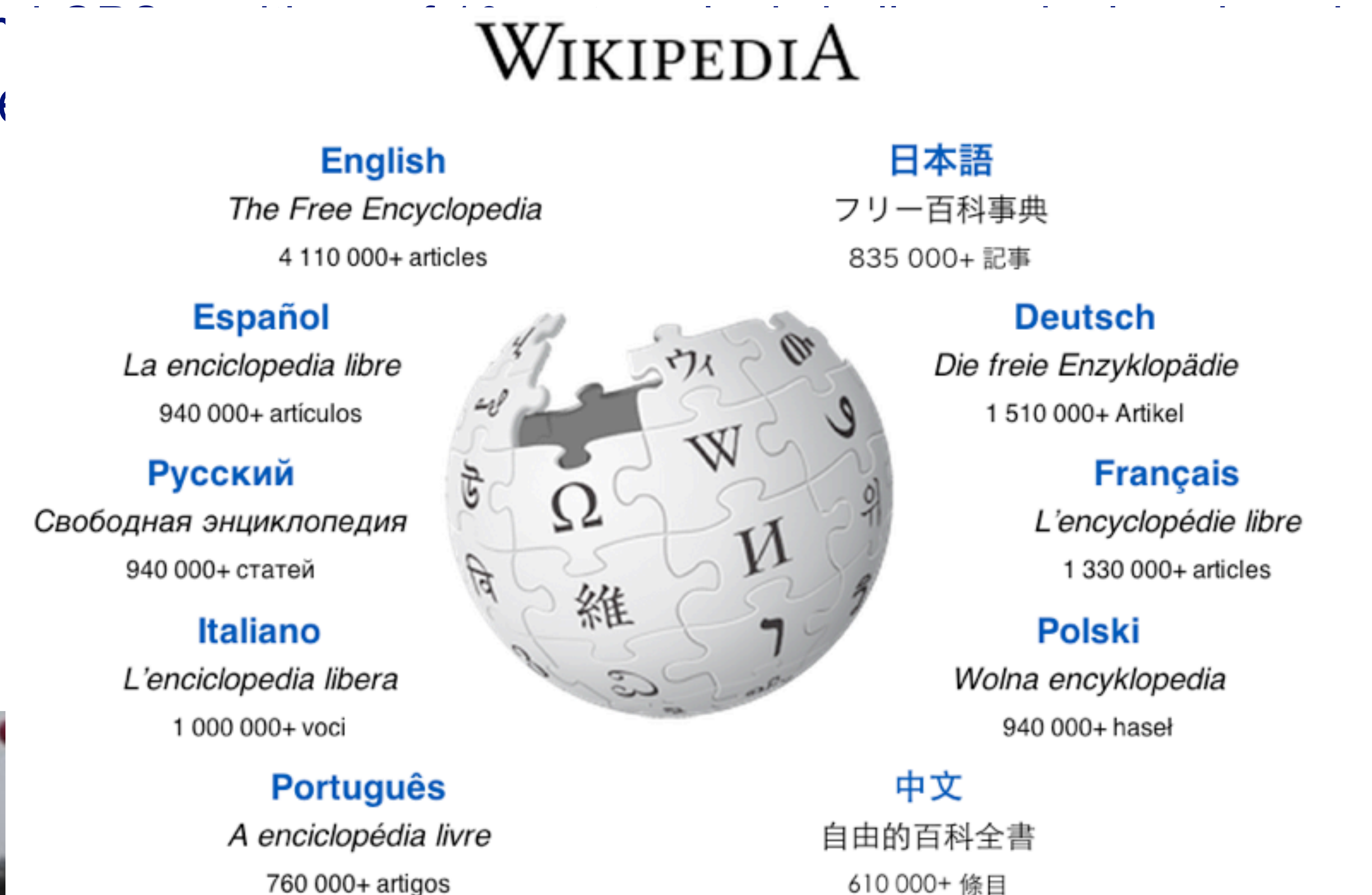
- From sensors
- From simulations
- From broad ranges of phenomena
- Over wide space and extended time
- Over masses of "*prosumers*"

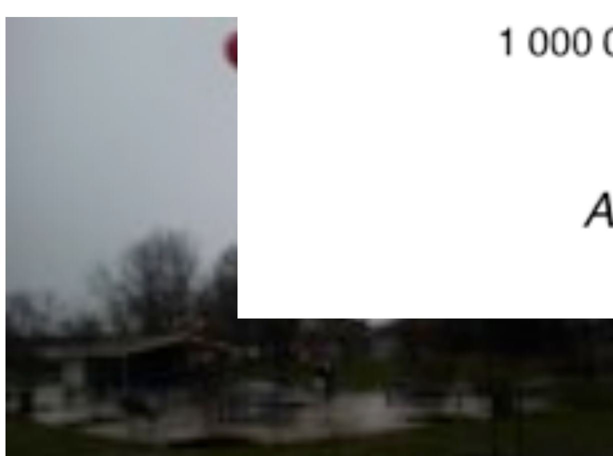
“Prosumers”

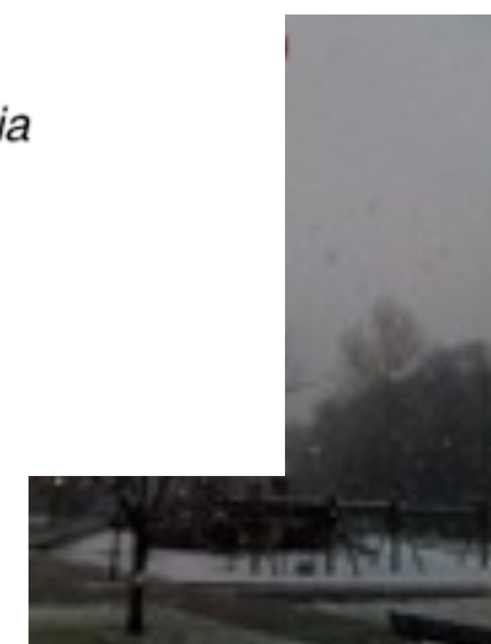
DARPA *Red Balloon Challenge* : 40 K$

Fir nly

ove







3. Massive Data Processing

What's new ?

a) **Scaling-up**

b) **Integration**

c) Automated processing and interpretation capabilities

- Automated search, mining
- Visualization

3. Massive Data Processing

What's new ?

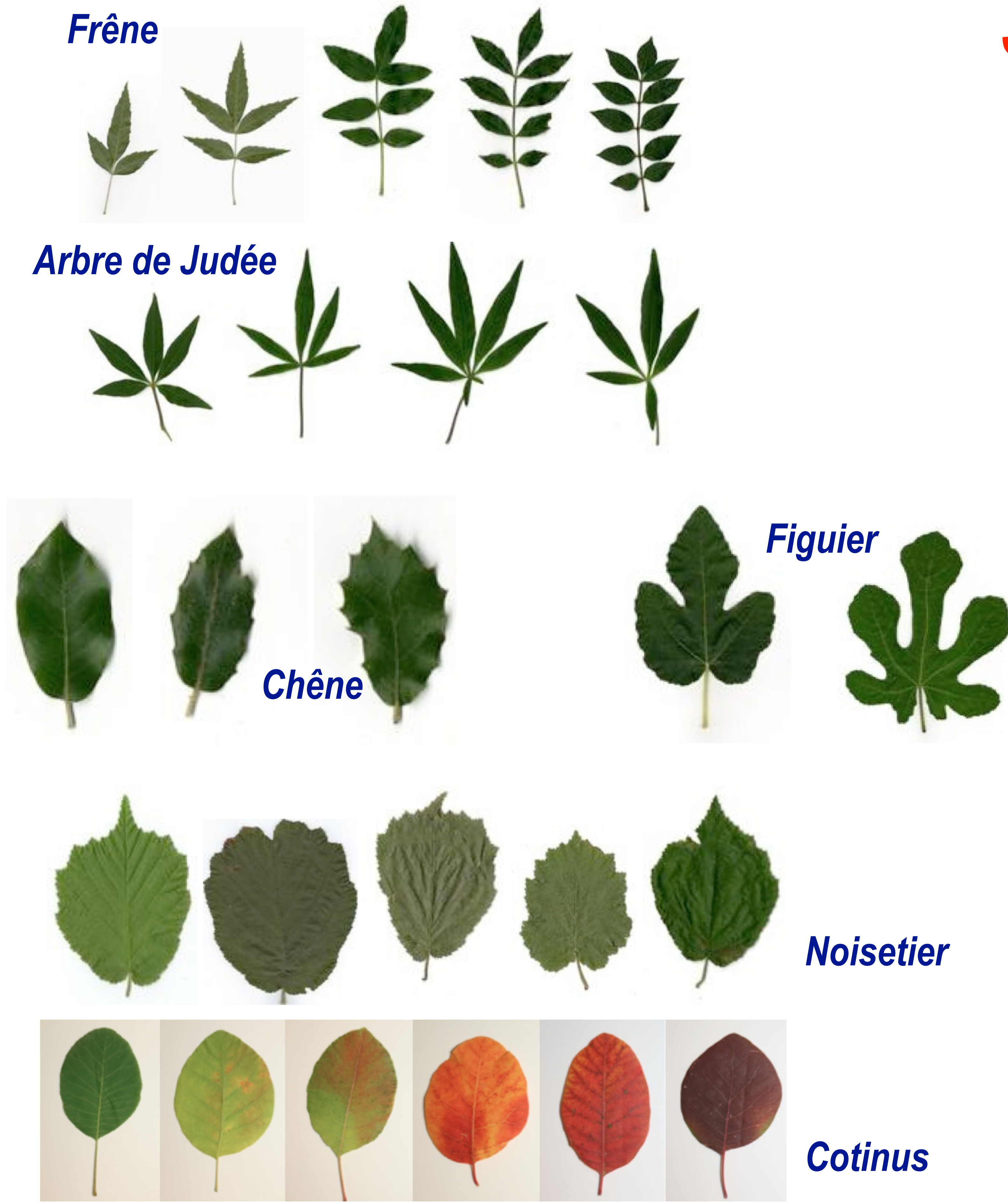
a) **Scaling-up**

b) **Integration**

c) Automated processing and interpretation capabilities

- Automated search, mining
- Visualization
- Machine learning techniques

Supervised learning



[Pl@ntNet]

Action recognition in images

Climbing

Action recognition in images

Reading

Cooking

Phoning

[Stanford Images test database]

3. Massive Data Processing

What's new ?

a) **Scaling-up**

b) **Integration**

c) Automated processing and interpretation capabilities

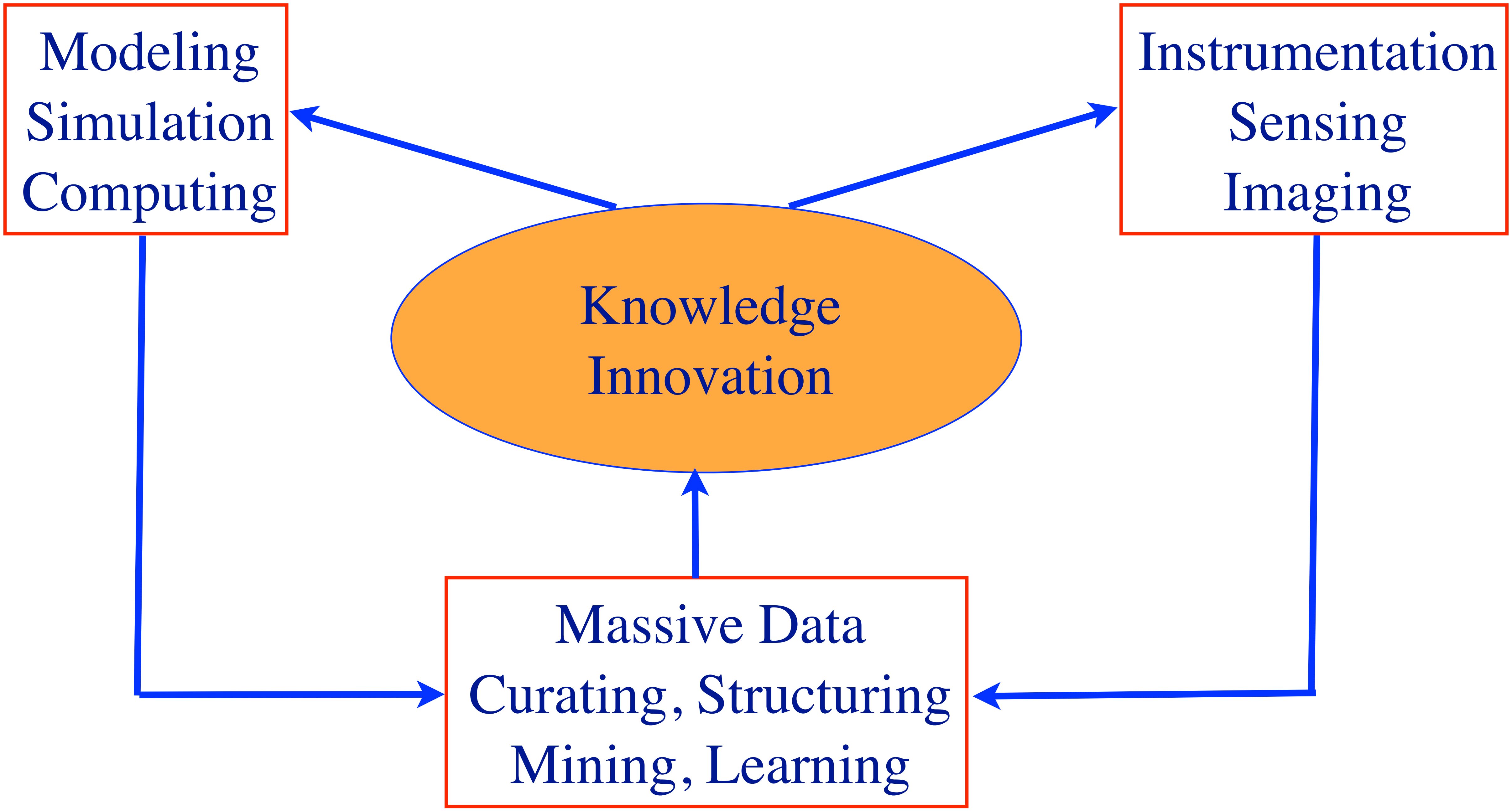
- Automated search, mining
- Machine learning techniques
- Semantic association

Data → Facts → Knowledge

Living organisms function according to protein circuits. Darwin's theory of evolution suggests that these circuits have evolved through variation guided by natural selection. The question of which circuits can so evolve in realistic population sizes and within realistic numbers of generations has remained essentially unaddressed.

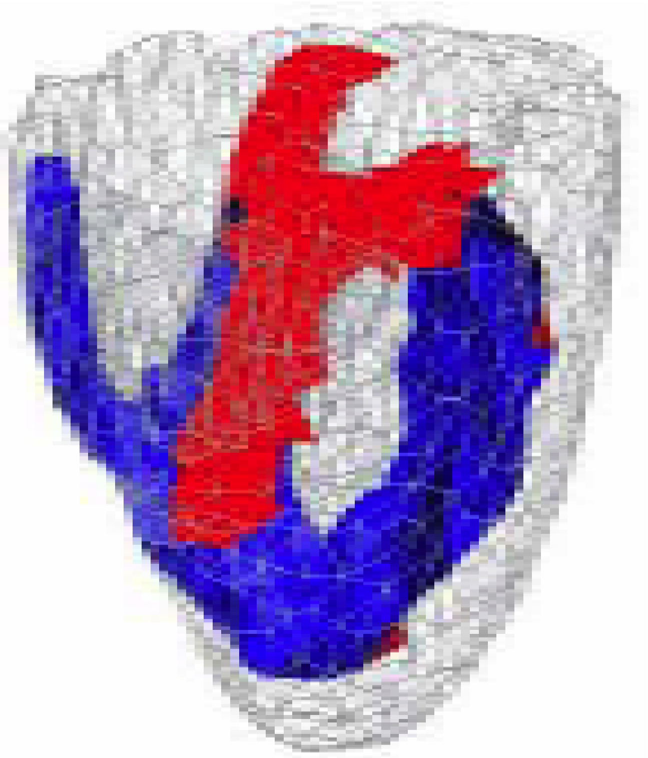
[Leslie Valiant]

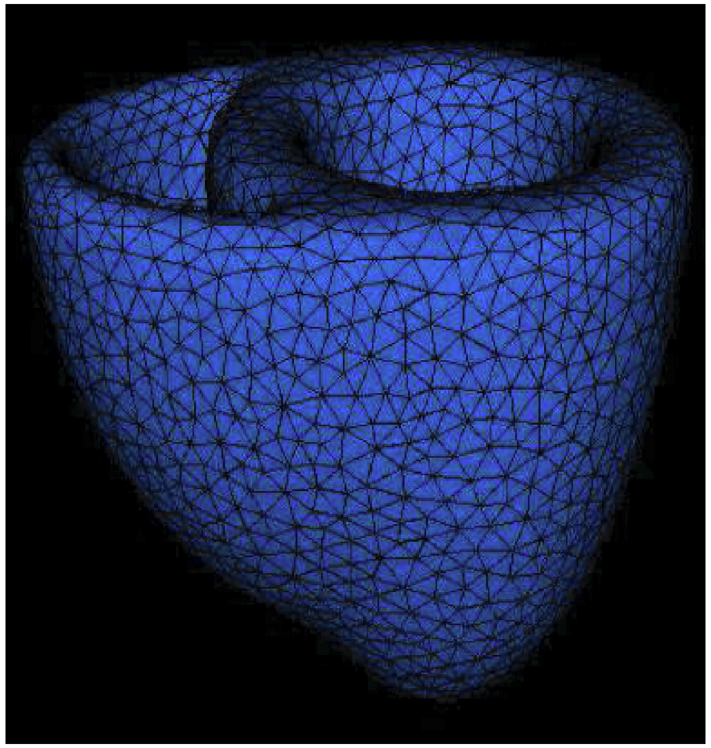
CSE Engines

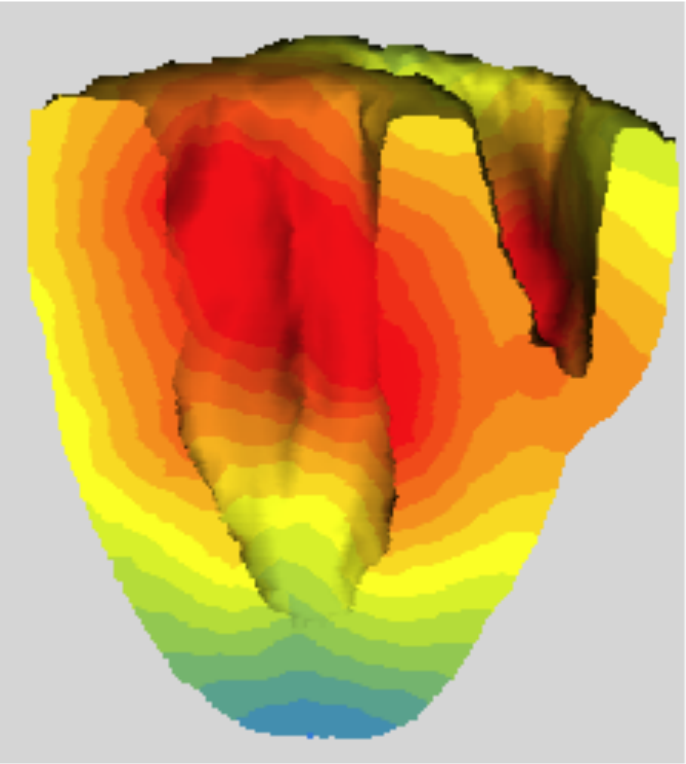

Modeling
Simulation
Computing
Instrumentation
Sensing
Imaging
Knowledge
Innovation
Massive Data
Curating, Structuring
Mining, Learning

Outline

- ✓ Motivations
- ✓ Ingredients
  1. Modeling, simulation and computing
  2. Instrumentation, sensing and imaging
  3. Massive data processing
- Impacts
  - Health and Life sciences
  - Earth and Environmental sciences
  - Physics, chemistry, material sciences
  - Engineering
  - Humanities and social sciences
- Conclusion

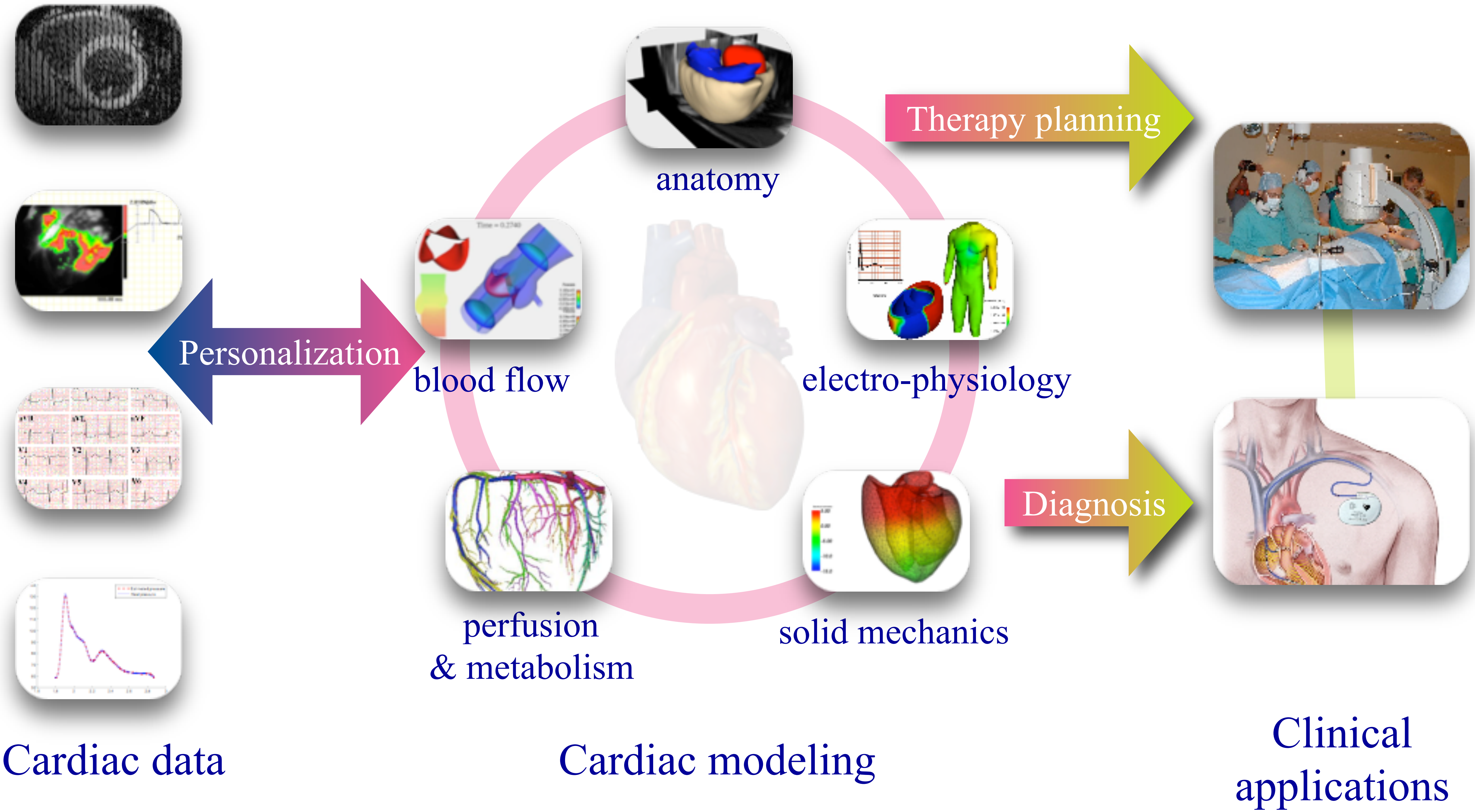






[CardioSence3D, Inria]

Health and Life Sciences



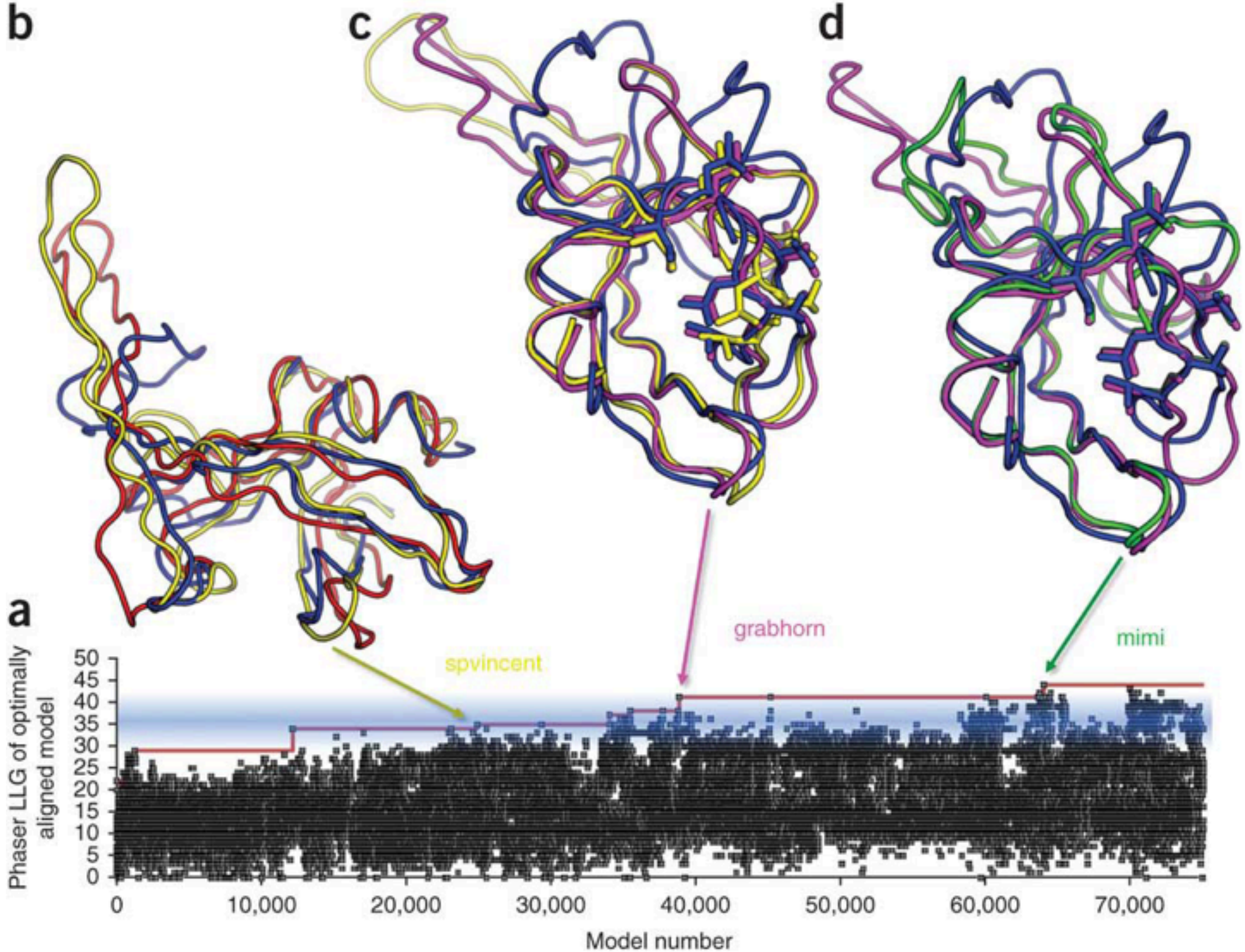
[CardioSence3D, Inria]

Health and Life Sciences

> Computer scientists may have the best skills to fight cancer in the next decade. Cancer is a genetic disease, caused by DNA mutations (whose) diversity within cancer type makes it so hard to eradicate

[D. Patterson, Berkeley]

- ***Algorithms***: develop efficient individual genome processing
- ***Machines***: Collect cancer genomes and disseminate widely
- ***People***: Explore the engagement of people



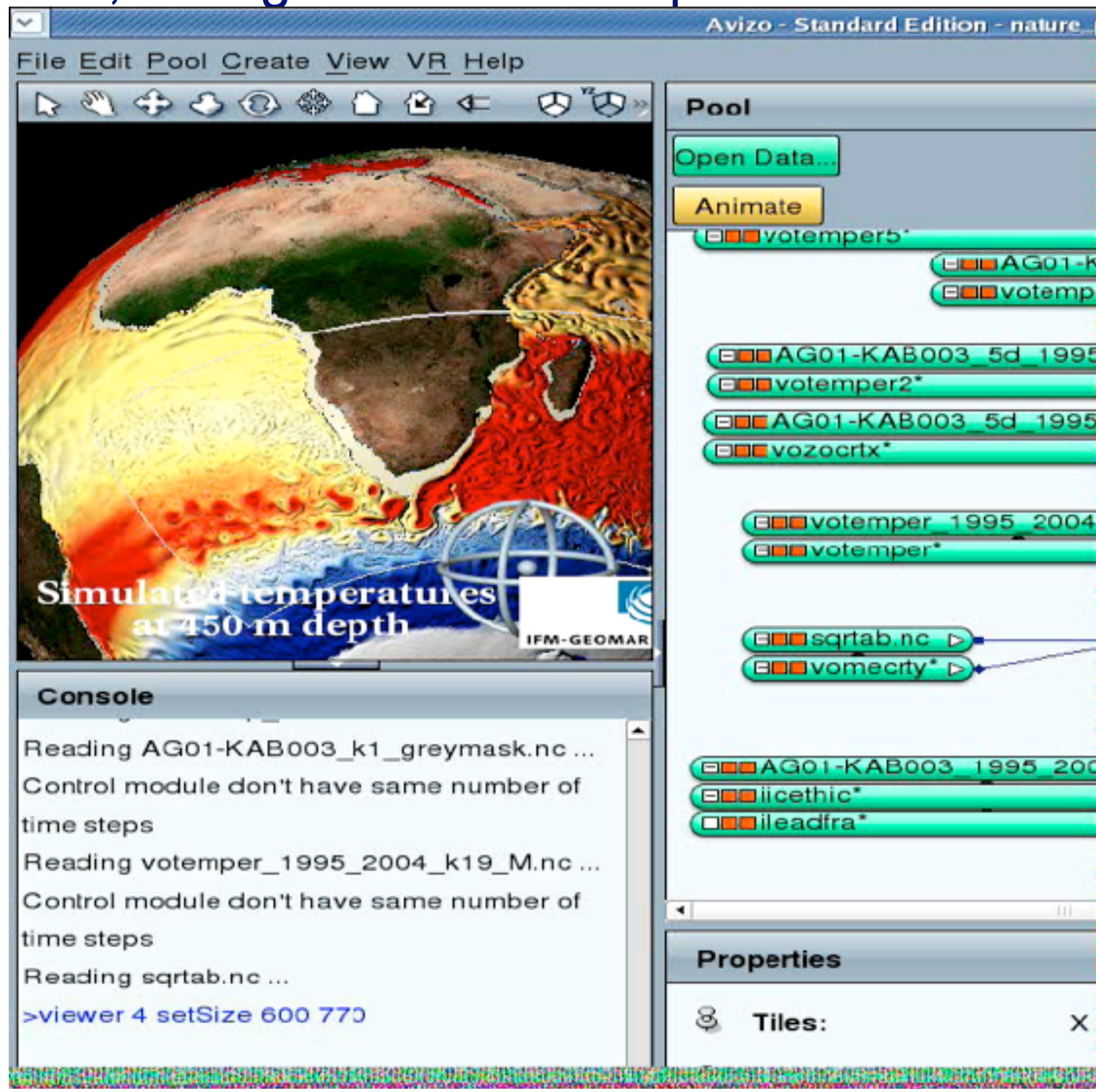
Crowd-sourcing discovery: Structure of the Mason-Pfizer protease retrovirus

[F.Khatib, Nature, Sept 2011]

Earth and Environmental Sciences

- Study of the bio-physical and social environments

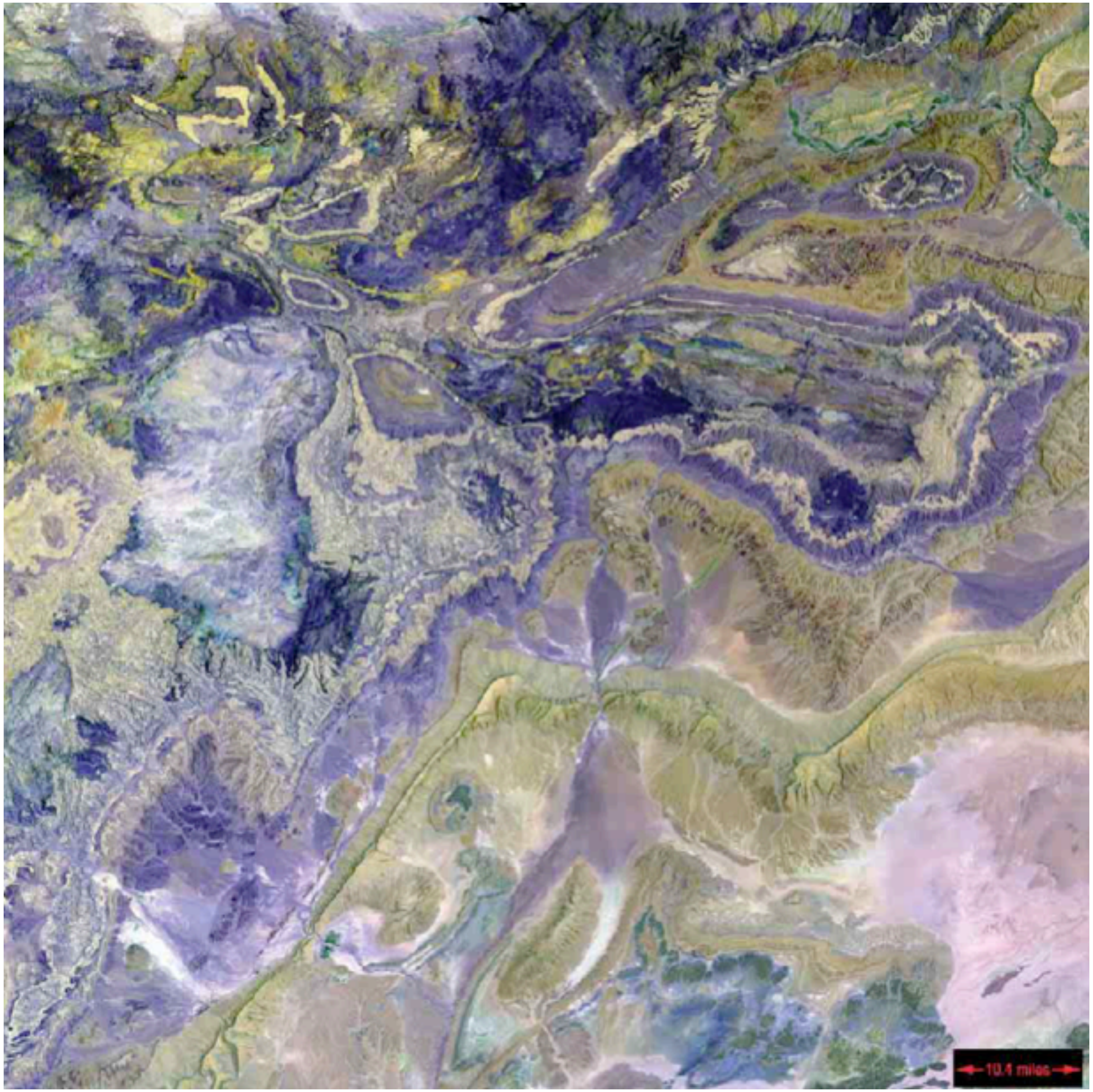
  Wide coupling between physical, biological and social phenomena



[E.Blayo, LJK/Inria]

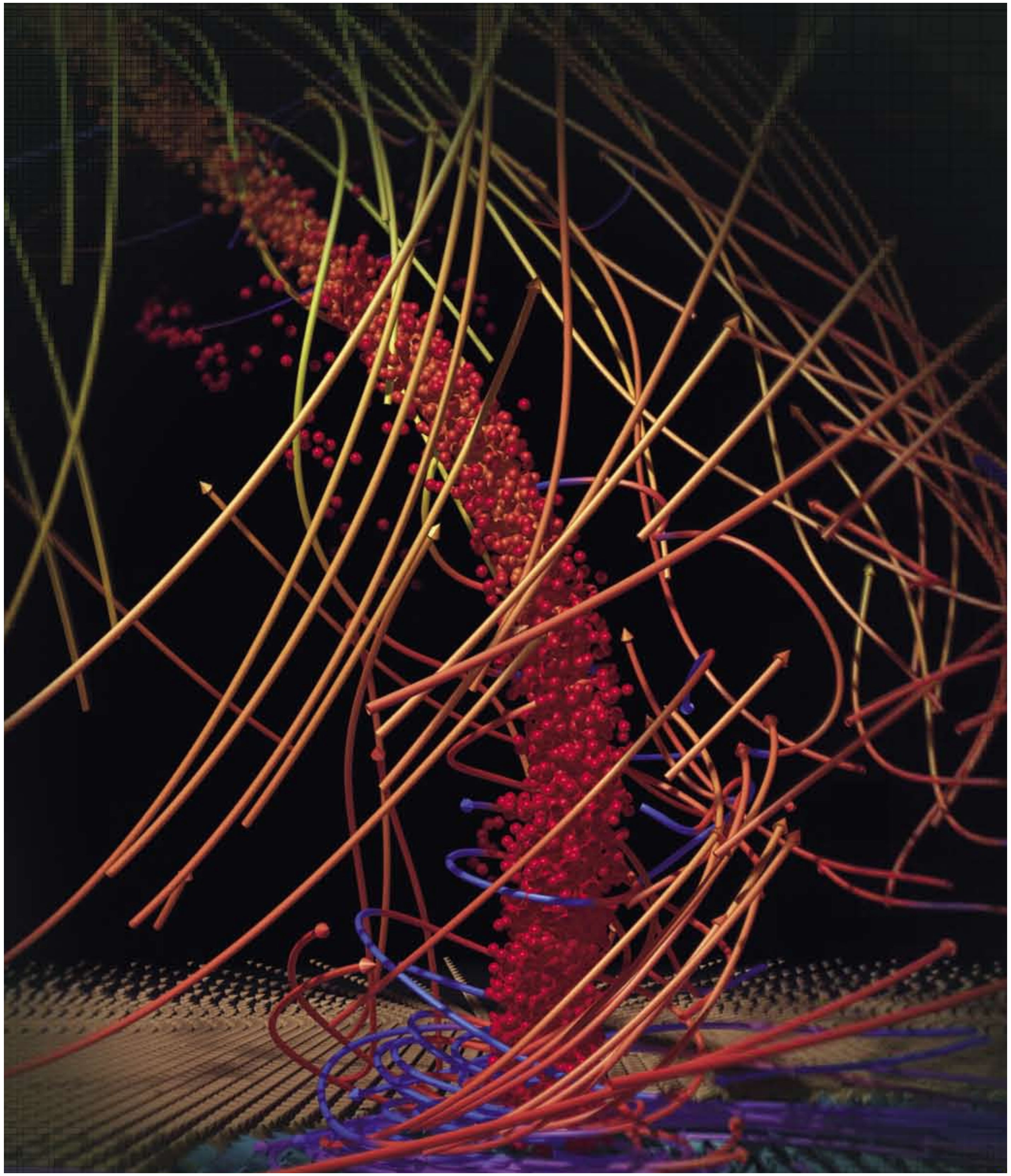
Earth and Environmental Sciences

Geological Survey of the Anti-Atlas, interferometer synthetic aperture radar (InSAR)



[H.B.Newman et al., CACM, 2003]

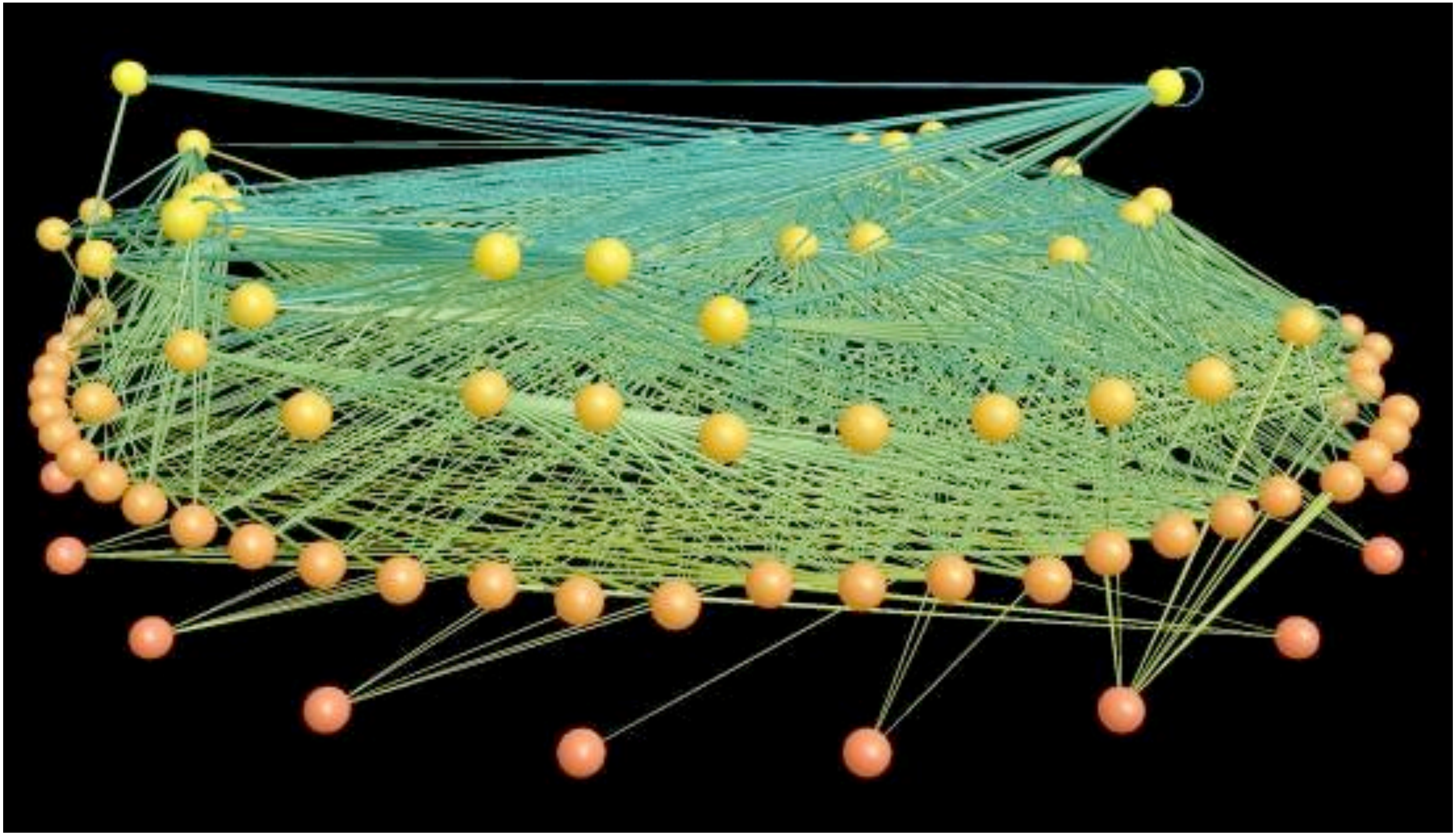
Earth and Environmental Sciences



[PITAC Report, 2005]

Tornado modeling and visualization

Feeding links among different trophic level species



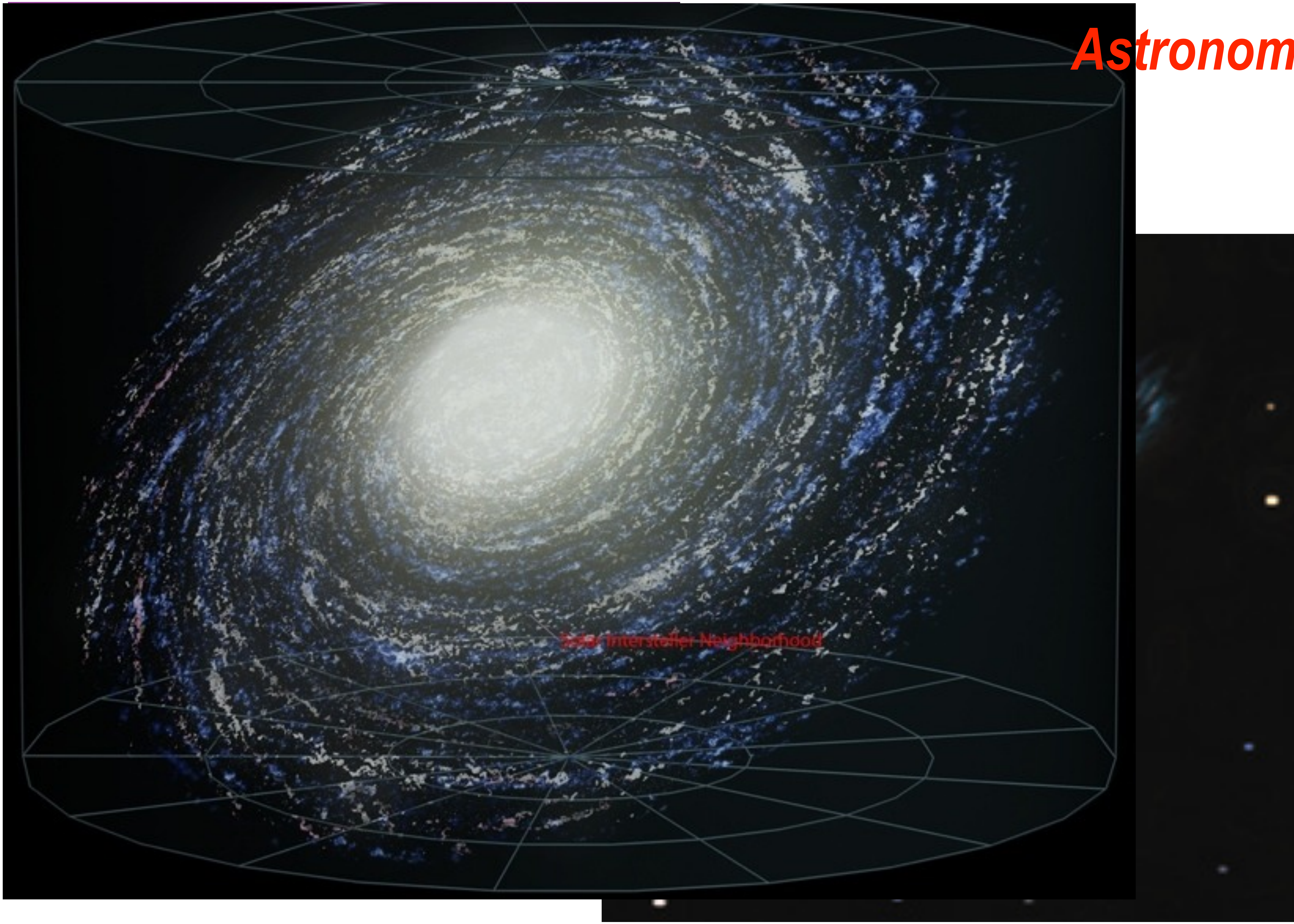
[M.Pascual, Comp. Biology, 2011]

Earth and Environmental Sciences

Plant growth modeling
and simulation

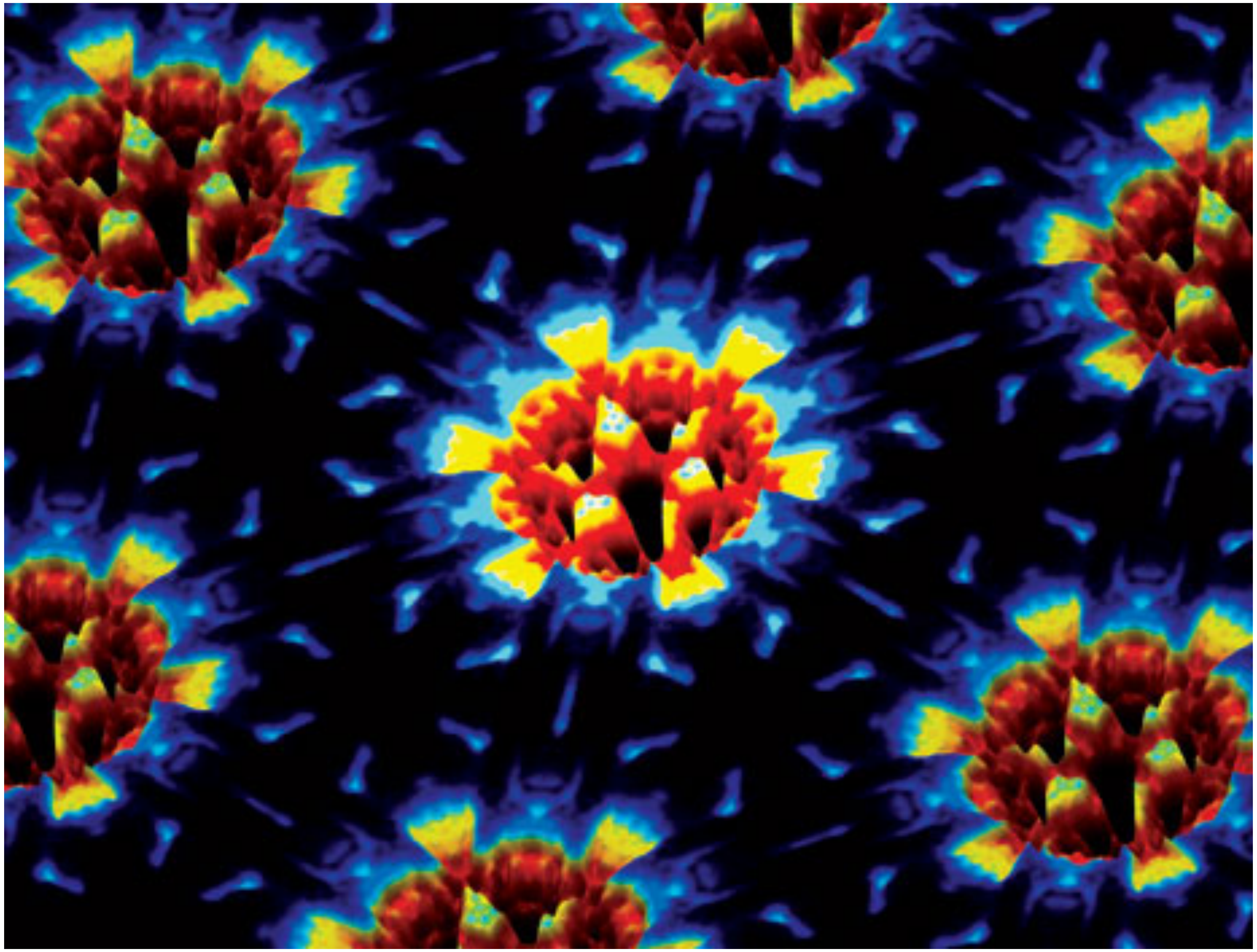
[Ph. de Reffye, Inria]

Astronomy



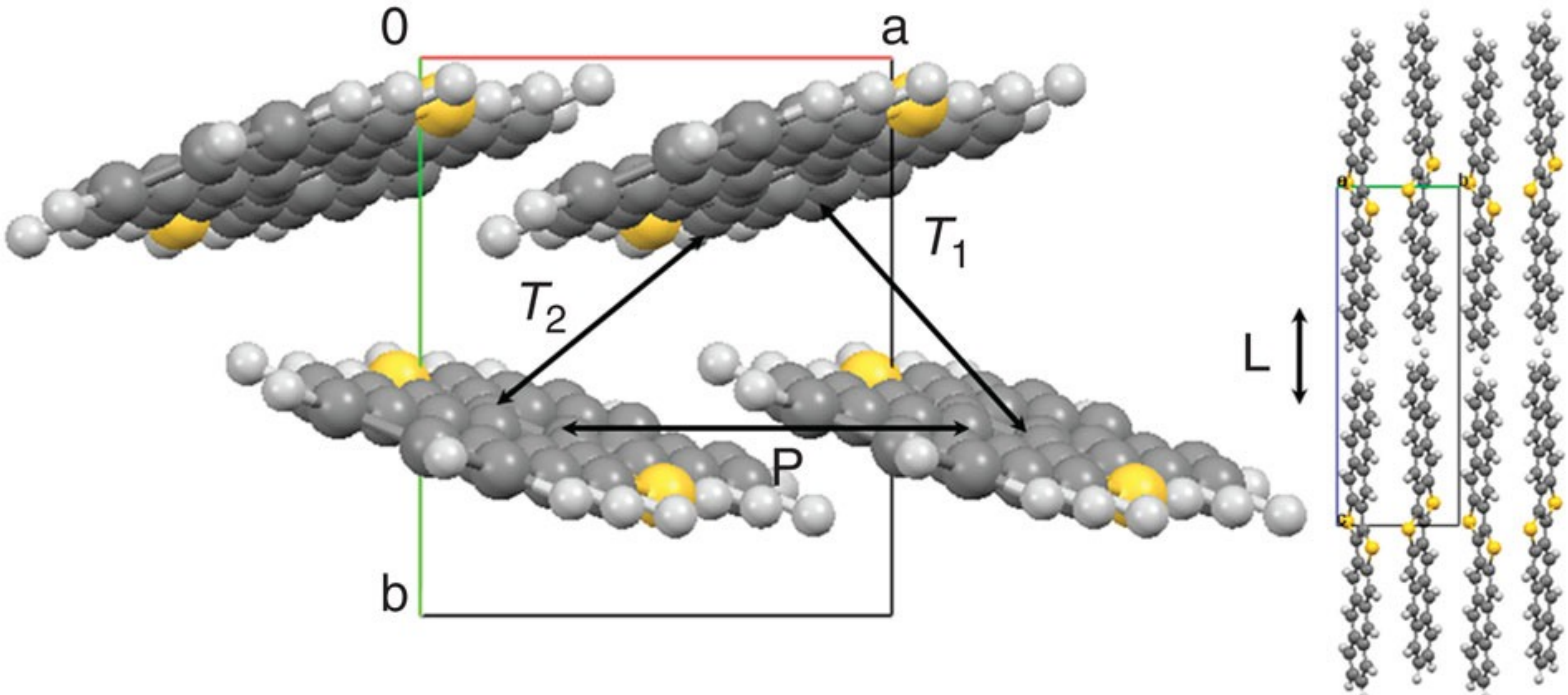
[L.Blitz, Scientific American, Oct.2011]

Computational model prediction of "topological insulators", with a follow up experimental confirmation



[J.E.Moore, IEEE Spectrum, July 2011]

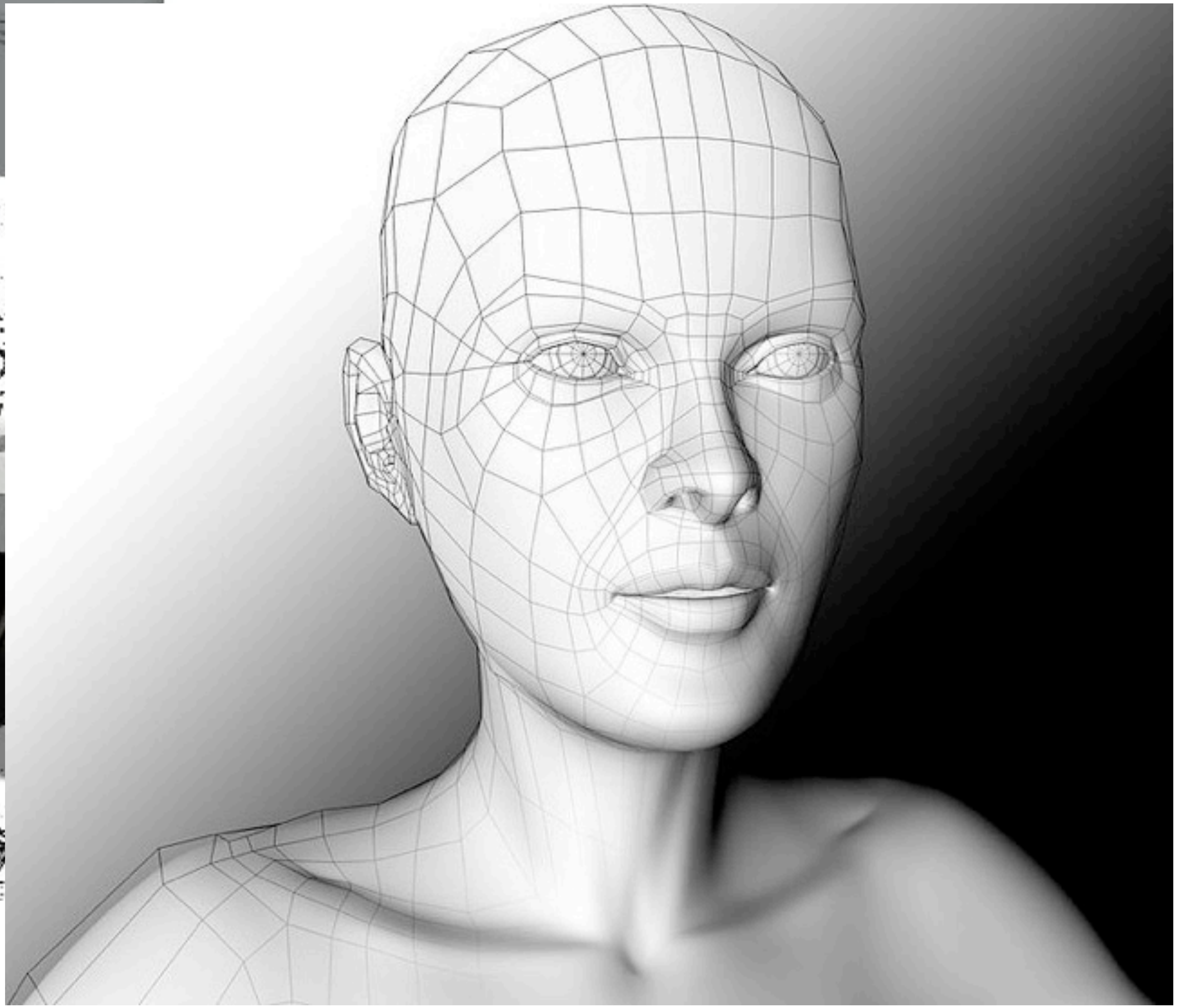
Screening techniques for the design of organic photovoltaic material: from computational discovery to experimental characterization of a high hole mobility organic crystal



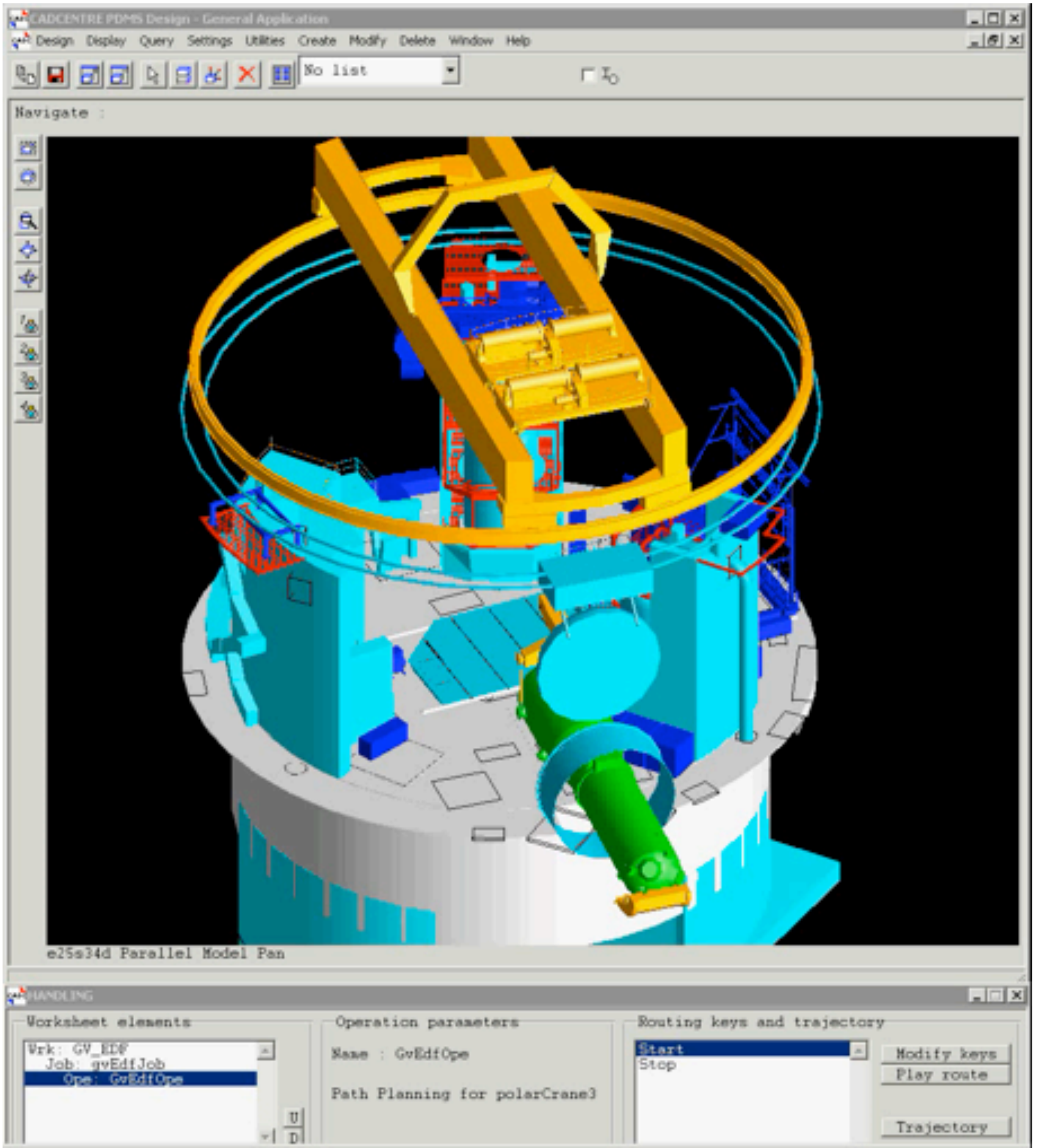
[A.Sokolov, Nature, Aug. 2011]

Engineering

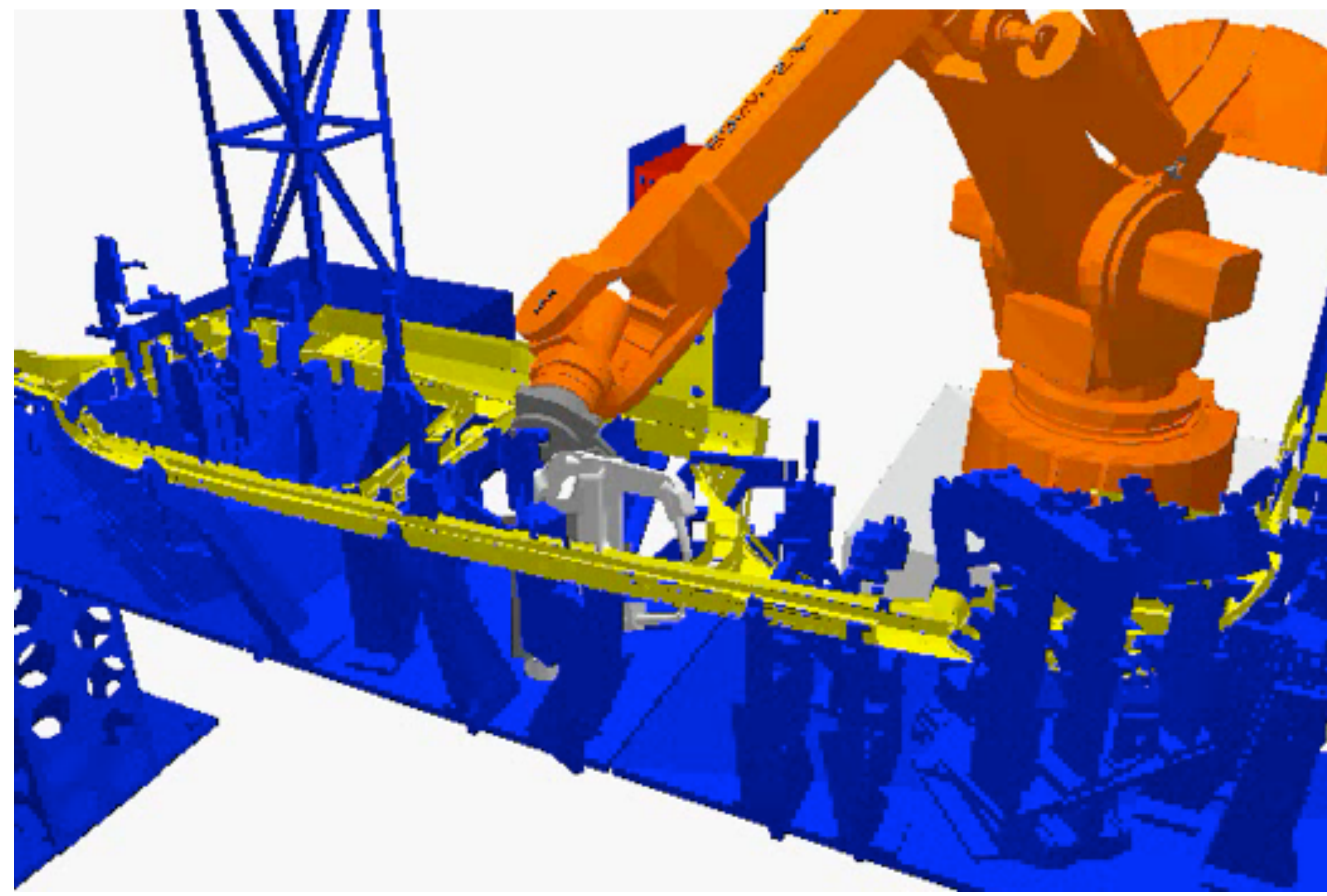
CAD-CAM models



Engineering

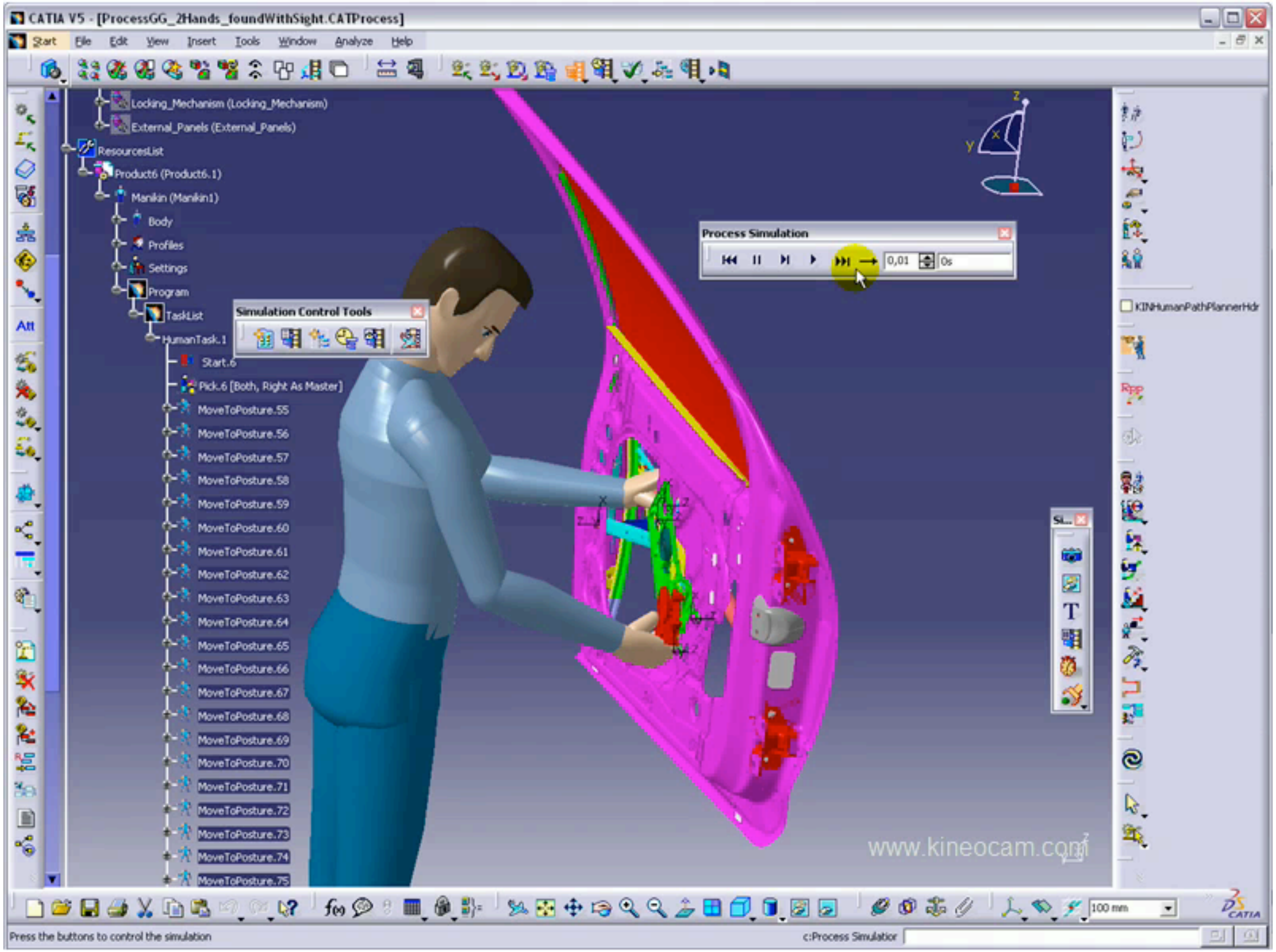


[J.Cortes, T.Siméon, LAAS]



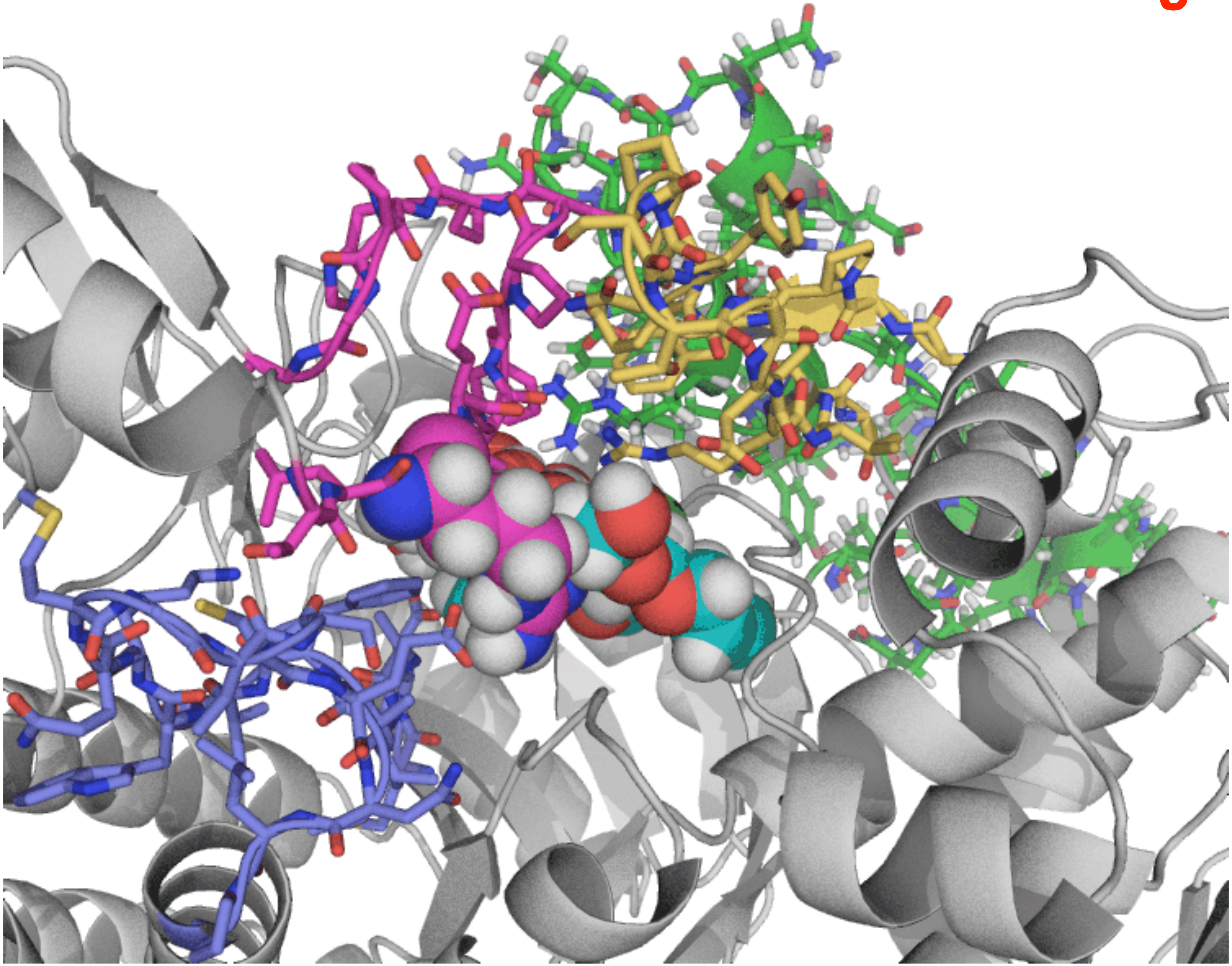
[Kineo]

Engineering



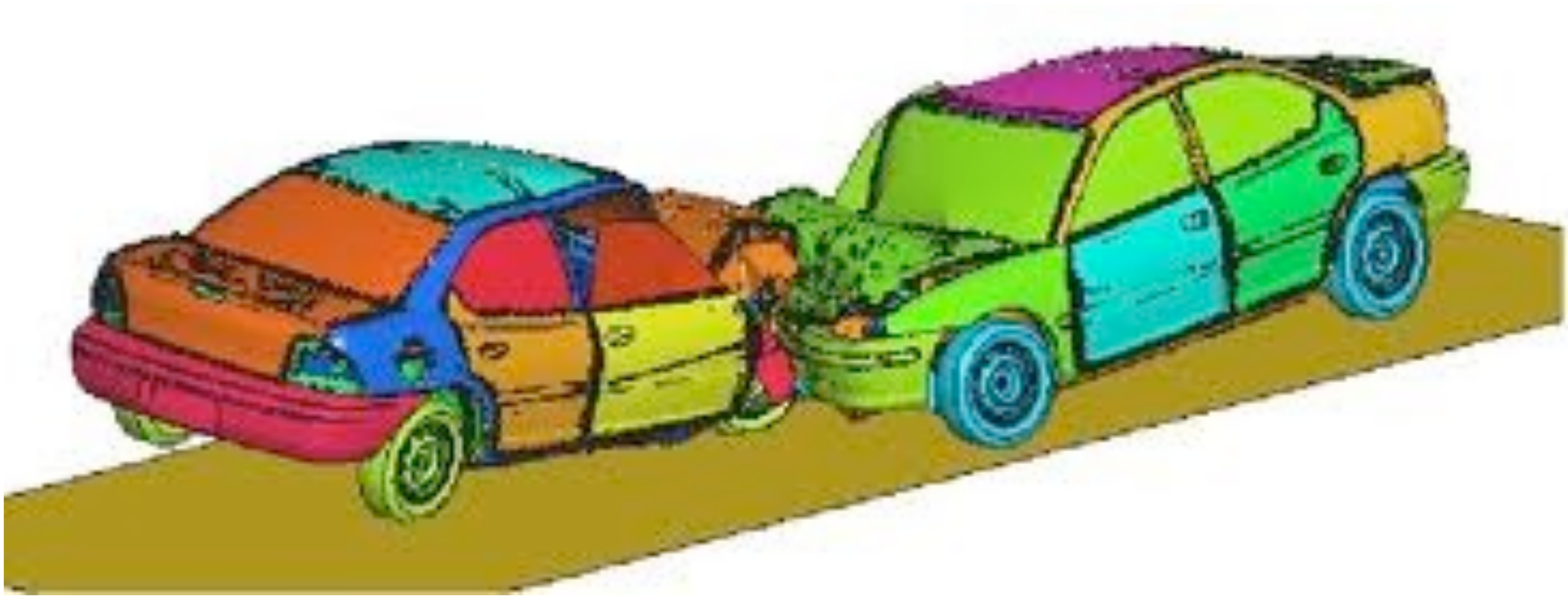
[Kineo]

Engineering

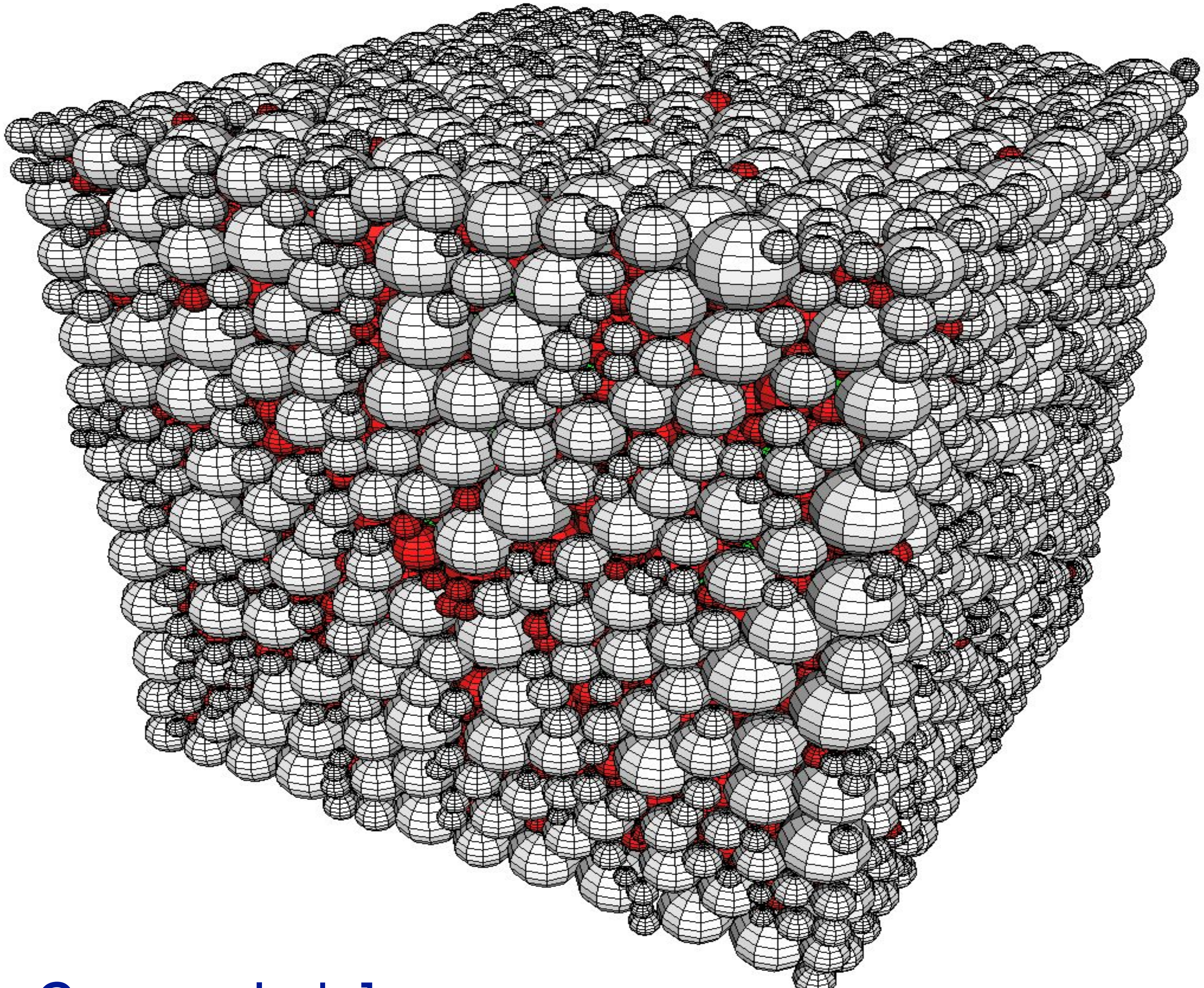


[J.Cortes, LAAS]

Stress models and simulations

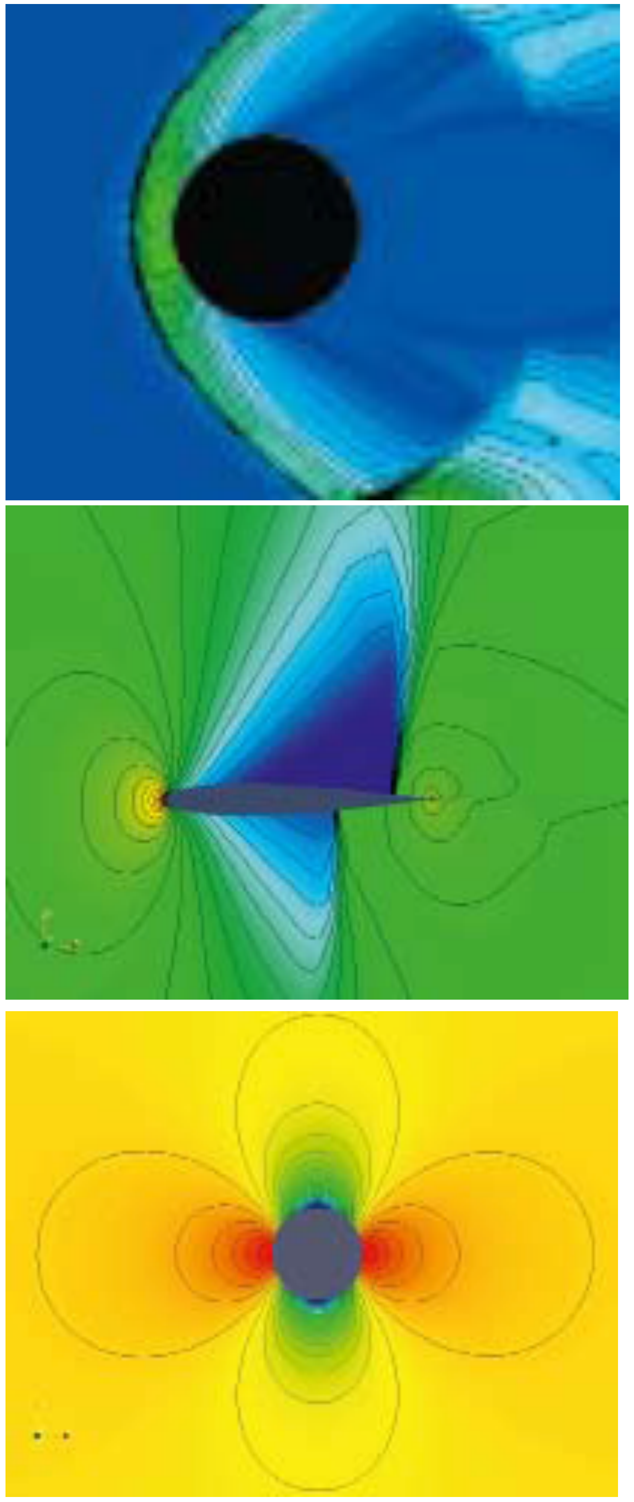


Material models



[P.L. George, Inria]

Aerodynamics models

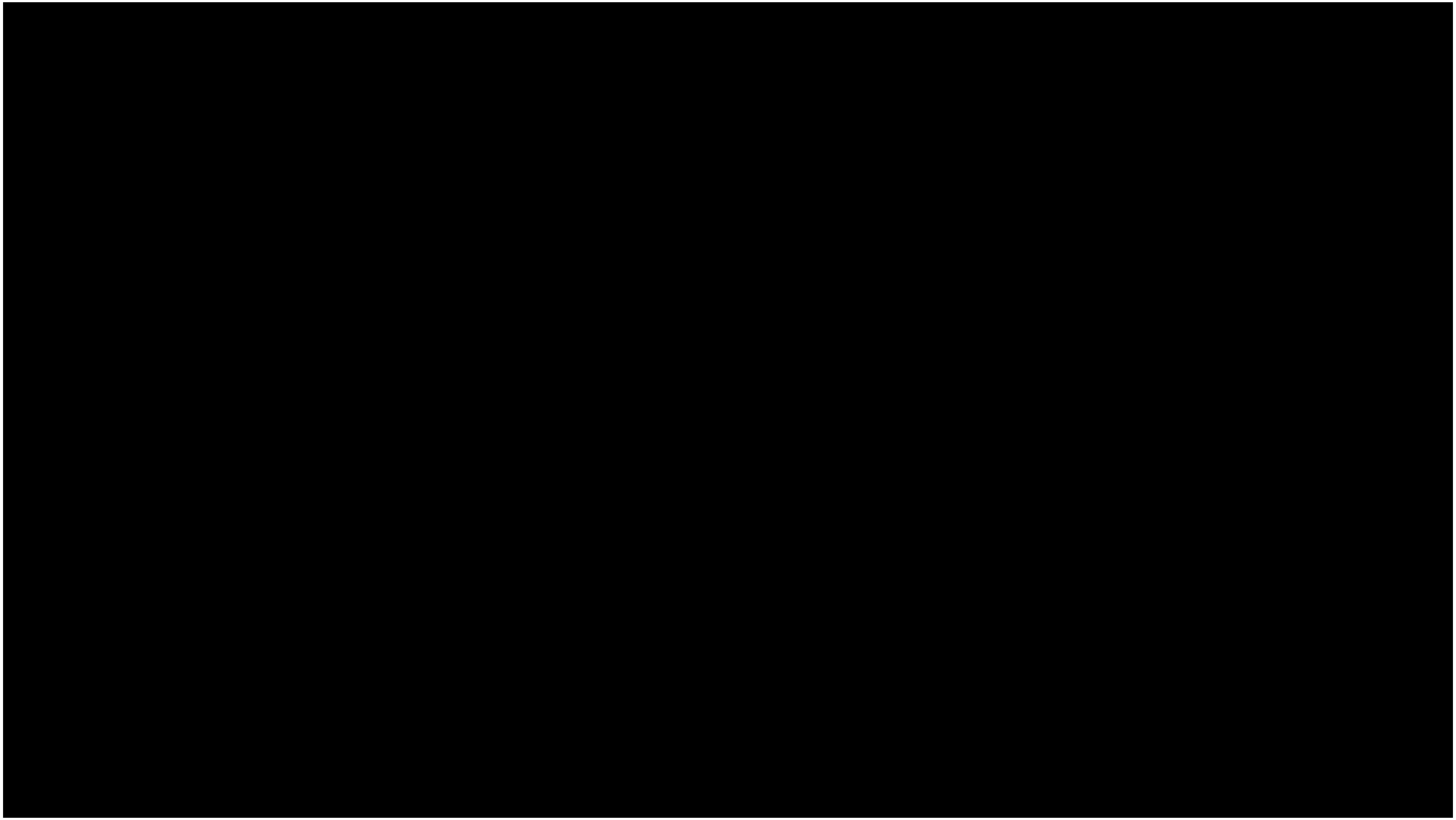


[R.Abgrall, Inria]

Software specification, formal proof and verification

[Airbus]

Helicopter Aerobatics Apprenticeship Learning



[U. Stanford]

Helicopter Aerobatics Apprenticeship Learning

Assume simple linear rigid dynamic models of helicopter

- Learn dynamic models, *one for each type of maneuver*
  - Regression from teacher's demonstrations
  - Improvement by reinforcement learning in autonomous flight
- Learn reference trajectories, one for each acrobatic figure
  - *Expectation-Maximization* on teacher's demonstrations
  - Temporal alignment and optimization
- Learn controllers, one for each acrobatic figure
  - *Differential dynamic programming*: solves continuous MDP's by iteratively approximating them as receding horizon LQR problems

Engineering

A350 Digital Mockup:
a virtual prototype

A380 Iron Bird:
a physical prototype

[Airbus]

Engineering

Design by ***incremental composition*** of numerical models of components

- Reduces cost and time for designing, engineering and prototyping
- Allows numerical exploration of numerous alternatives, including designs that appear a priori impossible
- Permits coordinated interdisciplinary contributions and uncoordinated anarchic contribution of crowd creativity
- Enables formal proofs of properties, realistic simulations, characterization and optimization

Engineering

Design by ***Integration of embedded*** actuators, sensors, processors and communication components as active and intelligent organs

- Creates new non functional properties: monitoring, diagnosis, recovery
- Brings new powerful performances and ***universal*** functionalities

Processors, computers, the web, (...) these new technologies have no specific use. Undifferentiated, universal, they transfer their utility project from the designer to the user. Those who design and produce them cannot predict to what nor to whom they will be useful. They have no direct finality. (...) Their functions are revealed posteriorly.

[M.Serres, Hominescence]

Social Sciences

- Social networks
- Web services over cell phones
- Computational macro-economy models
- Opinion space
- Media and documents analysis

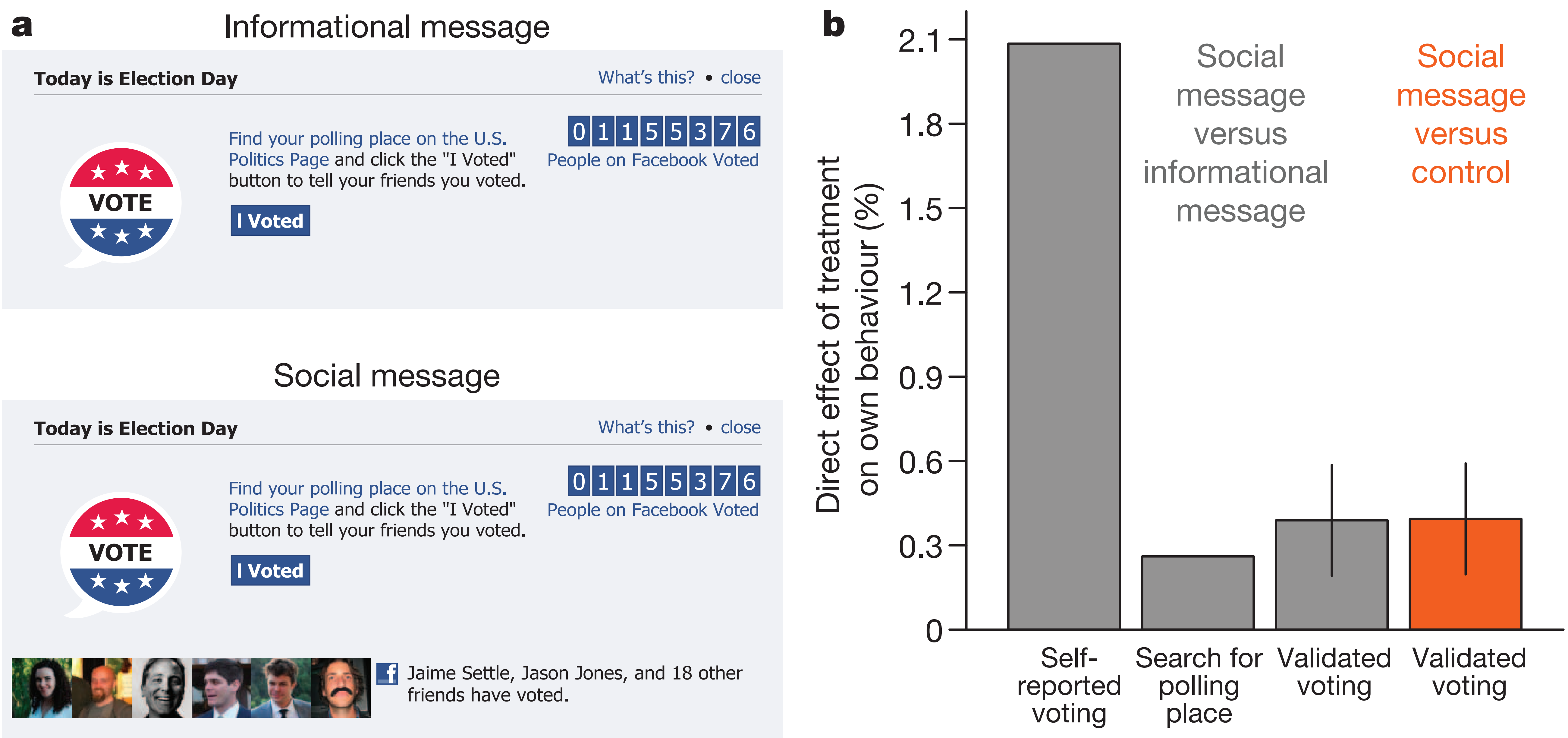
E-Democracy ?

[K.Goldberg, Berkeley]

Influential people

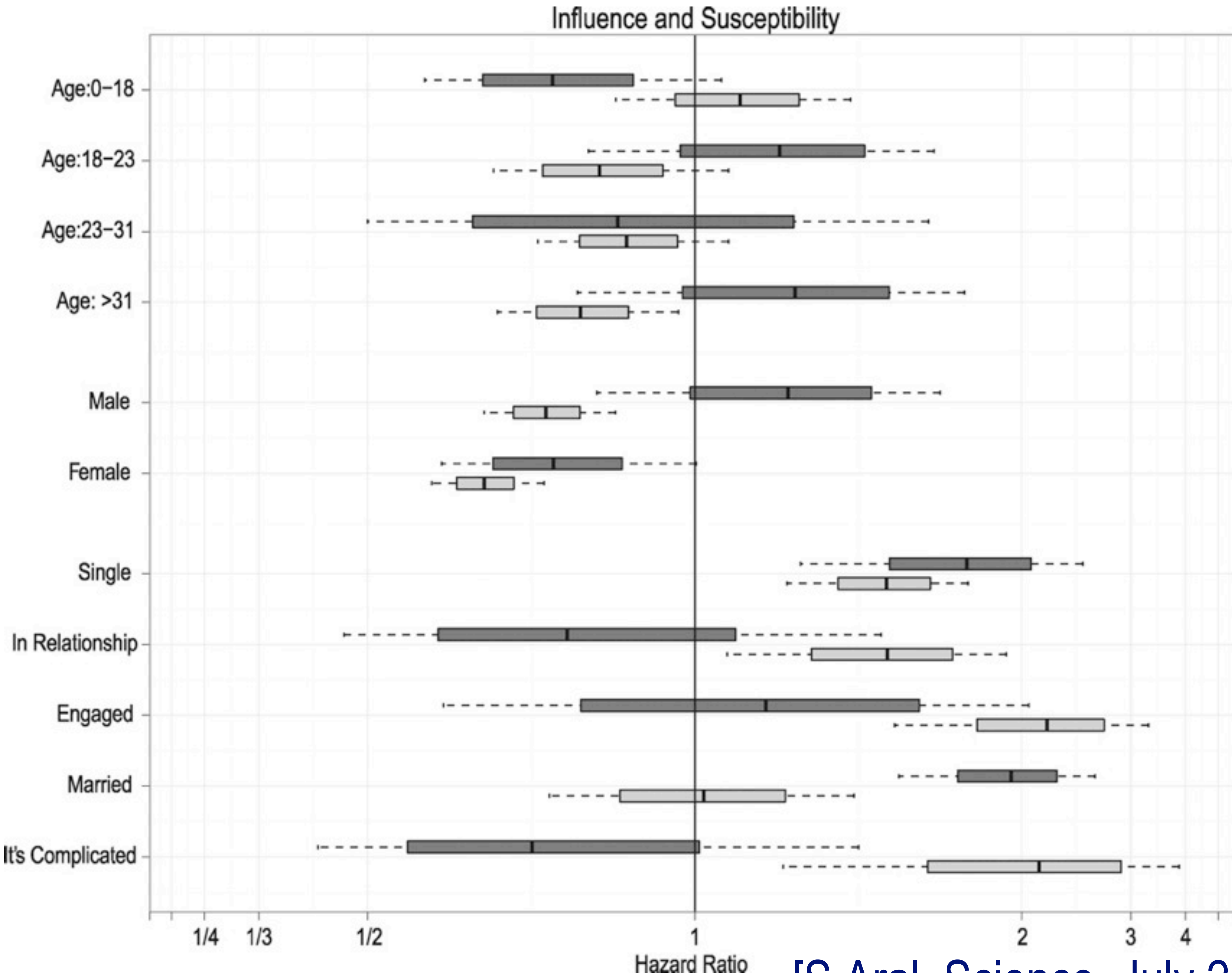
Peer influence in social networks

Study involving 61 Million people on Nov. 2010 US congressional elections



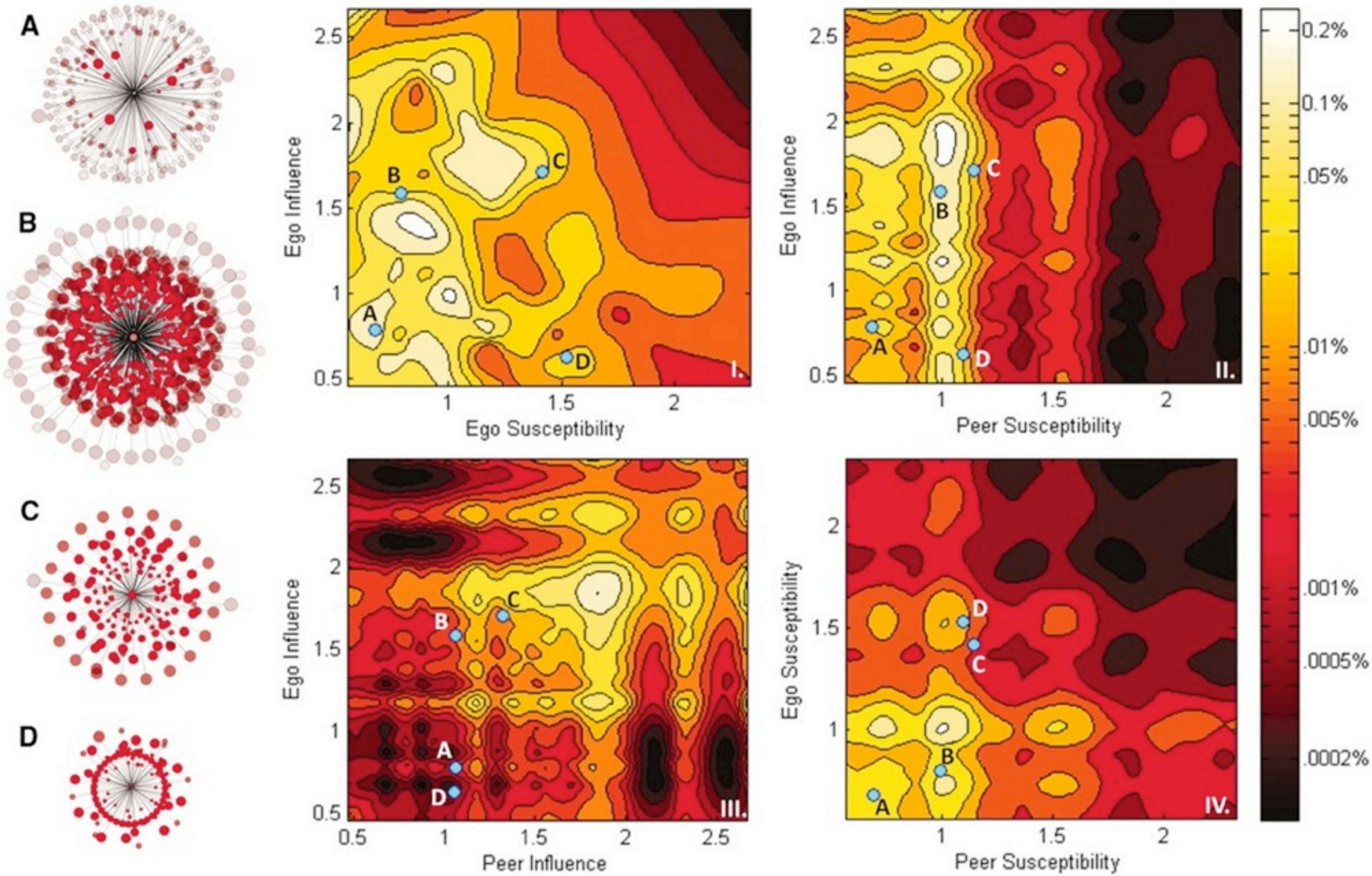
[R.Bond, Nature, Sept.2012]

Peer influence vs susceptibility in social networks

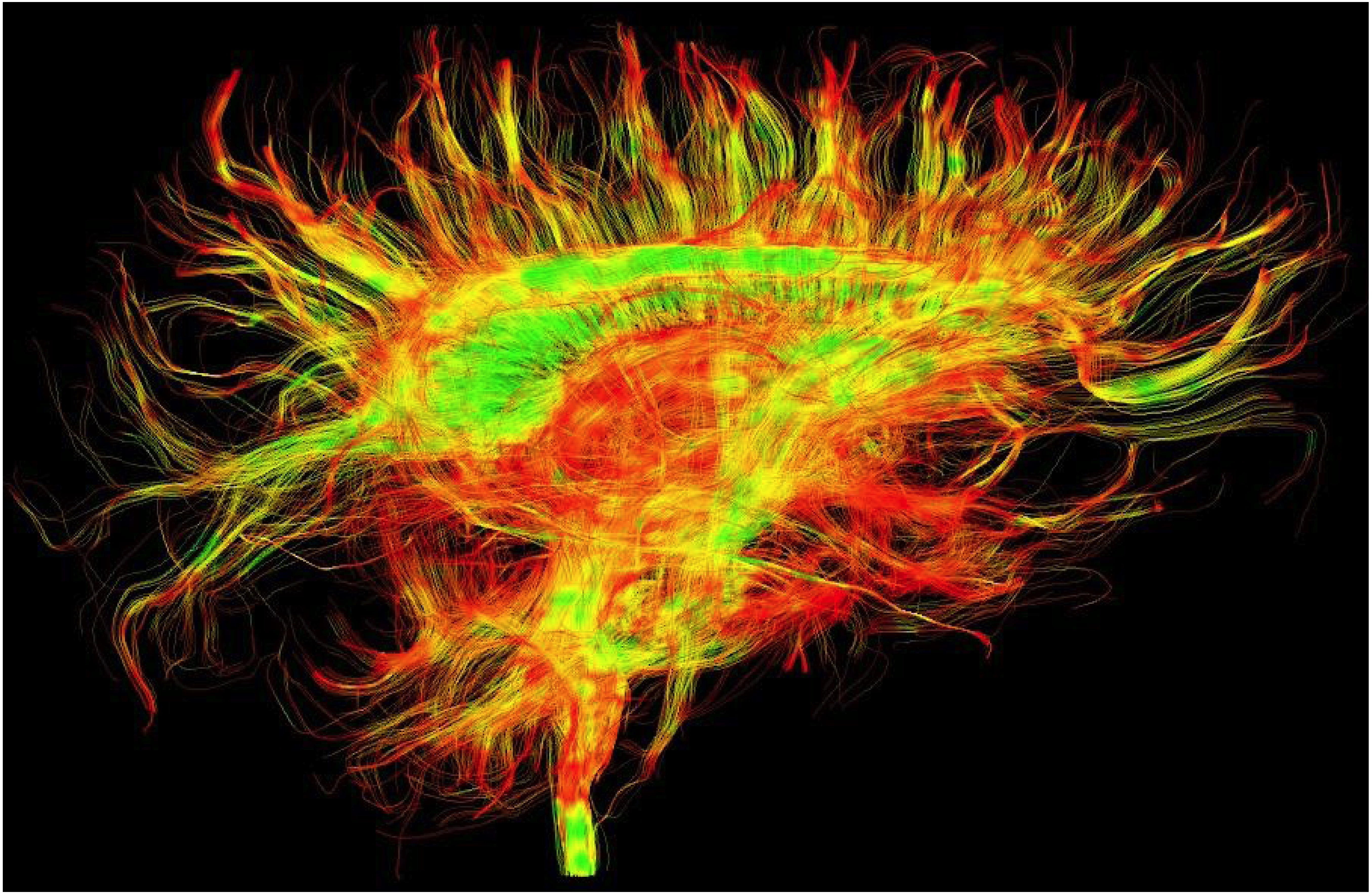


[S.Aral, Science, July 2012]

Joint distribution of influence and susceptibility

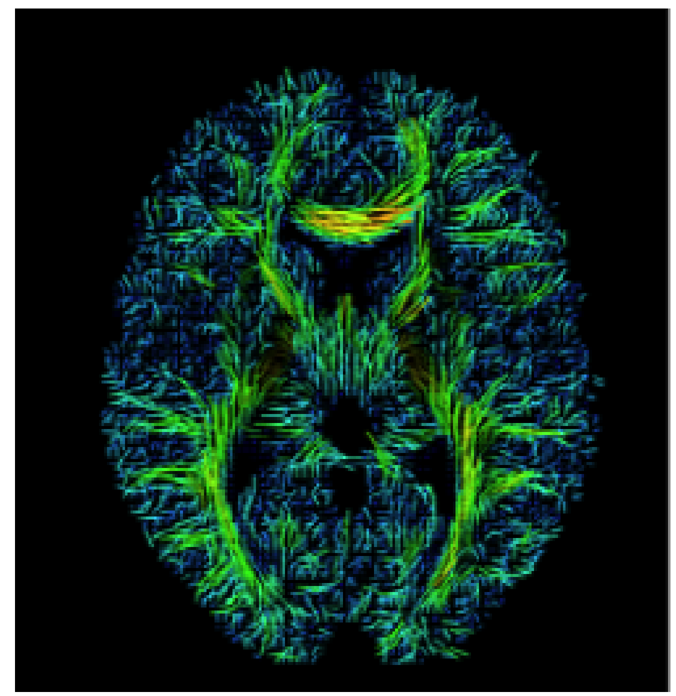


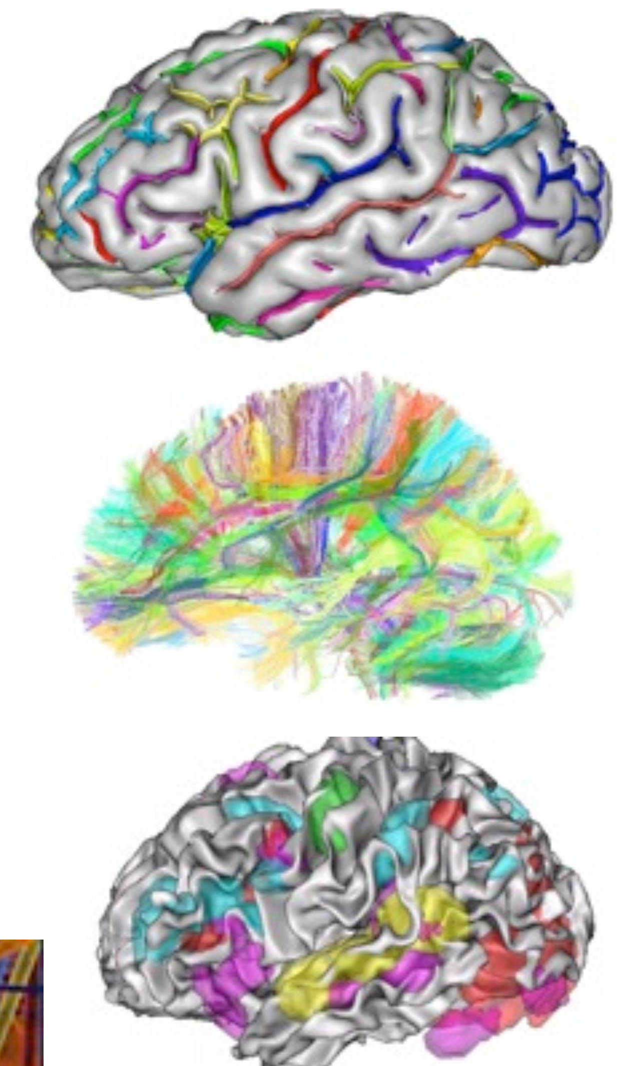
[S.Aral, Science, July 2012]



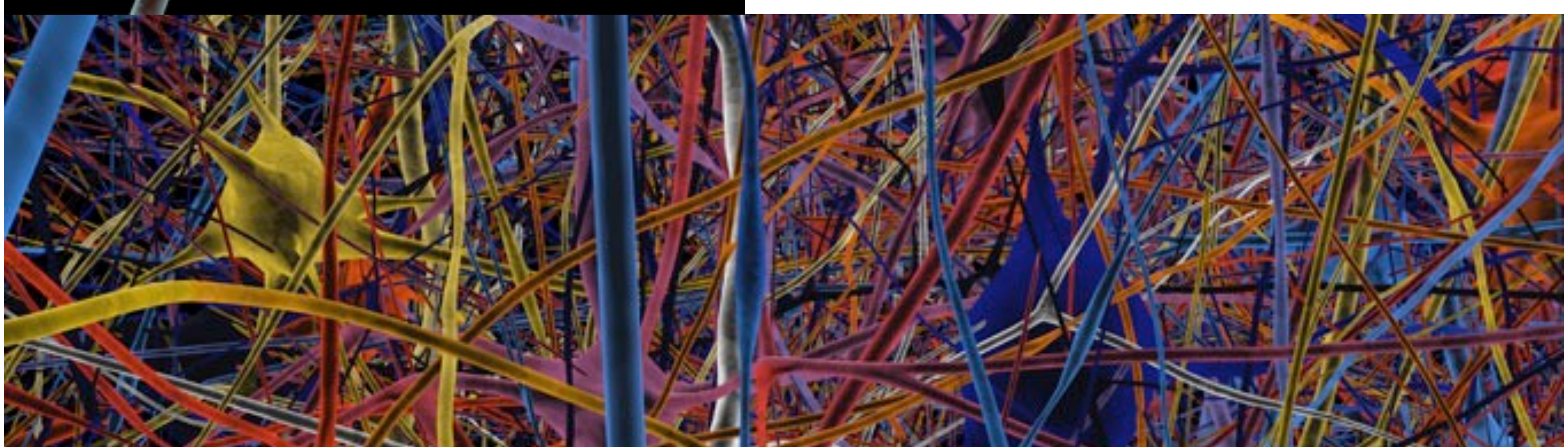
HBP
The Human Brain Project

EU Flagship Project





[Parietal, Inria]



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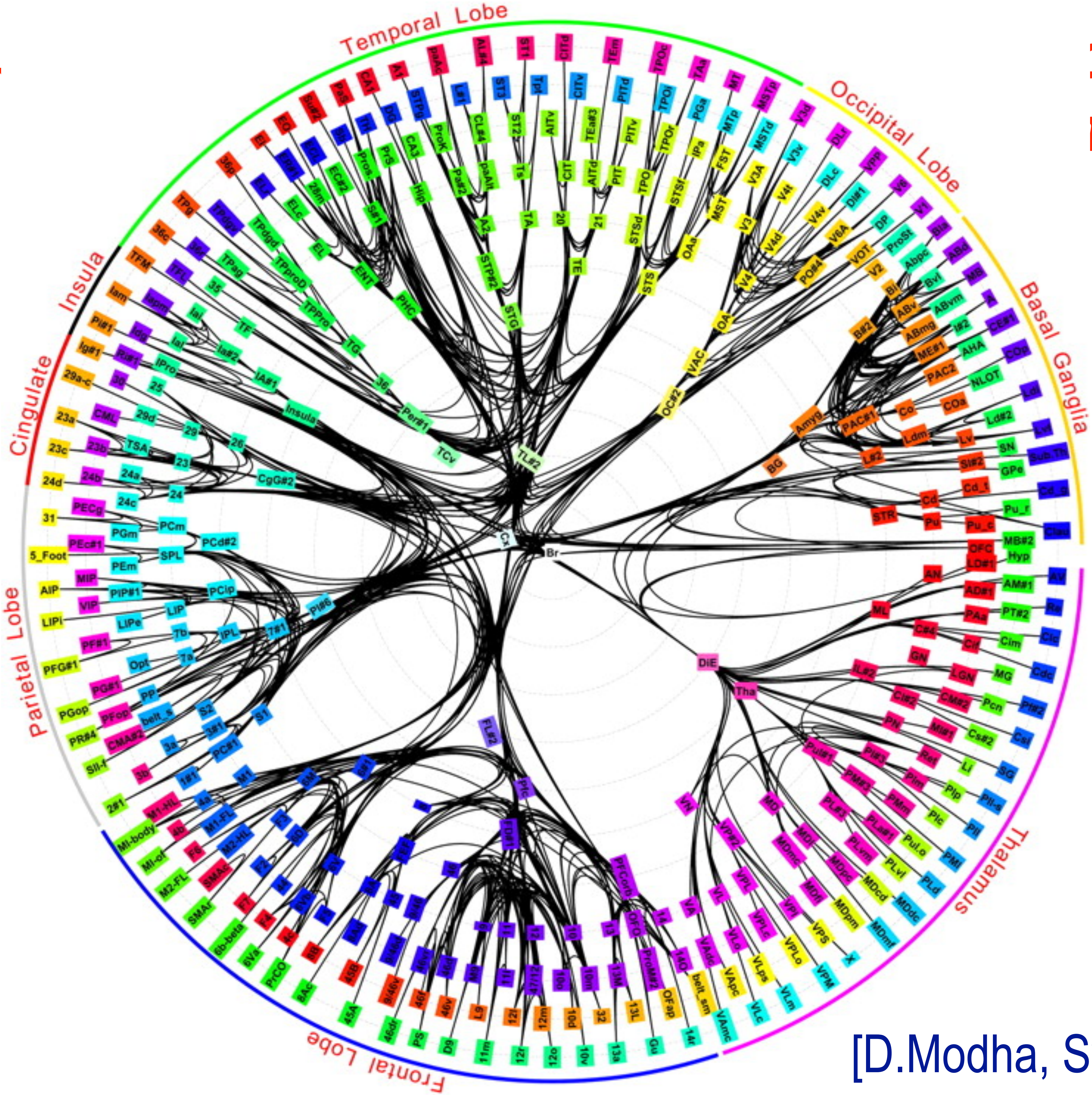
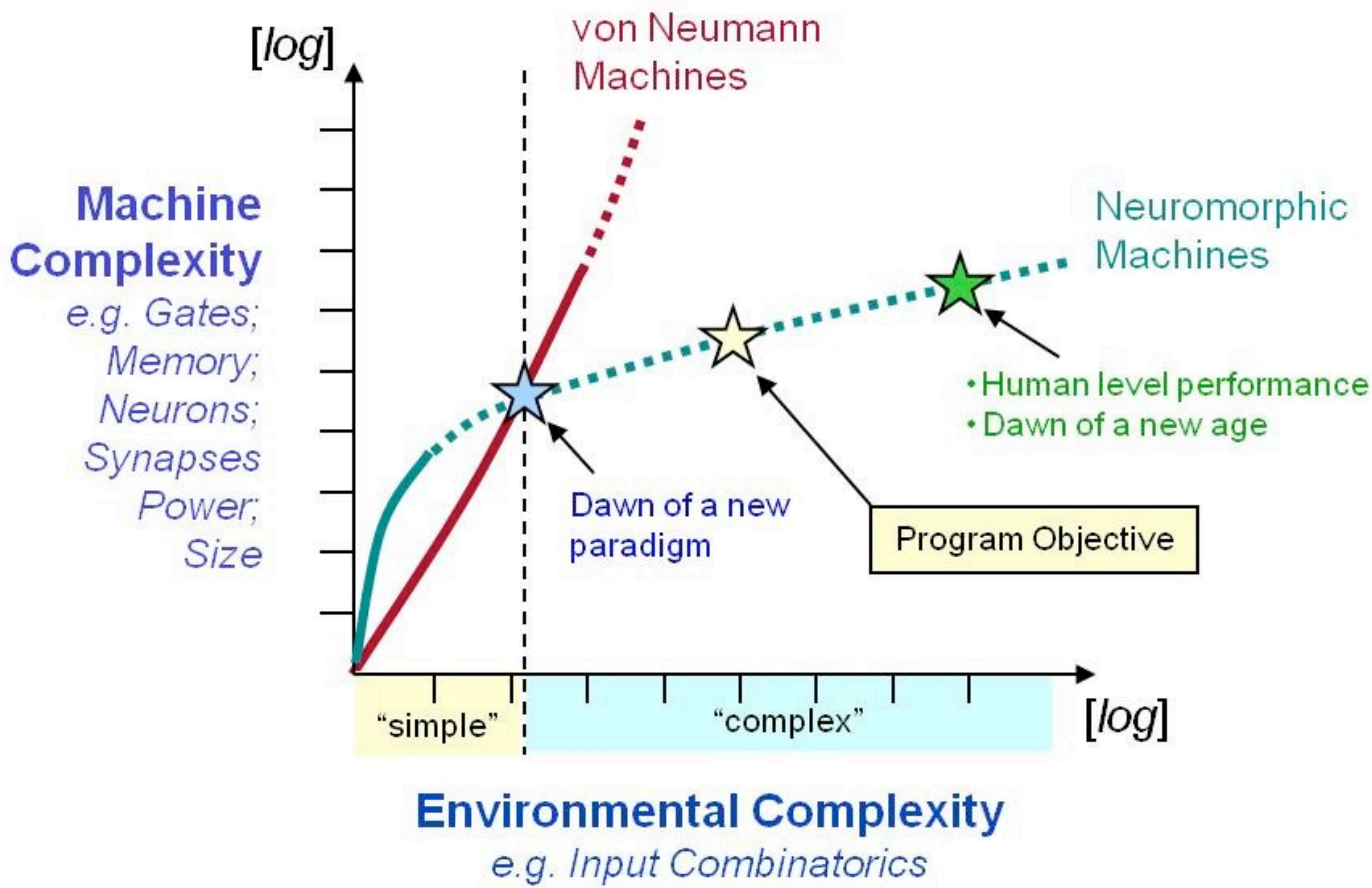


[D.Modha, SyNAPSE]

A scalable simulator for an architecture for Cognitive Computing



[D.Modha, SyNAPSE]

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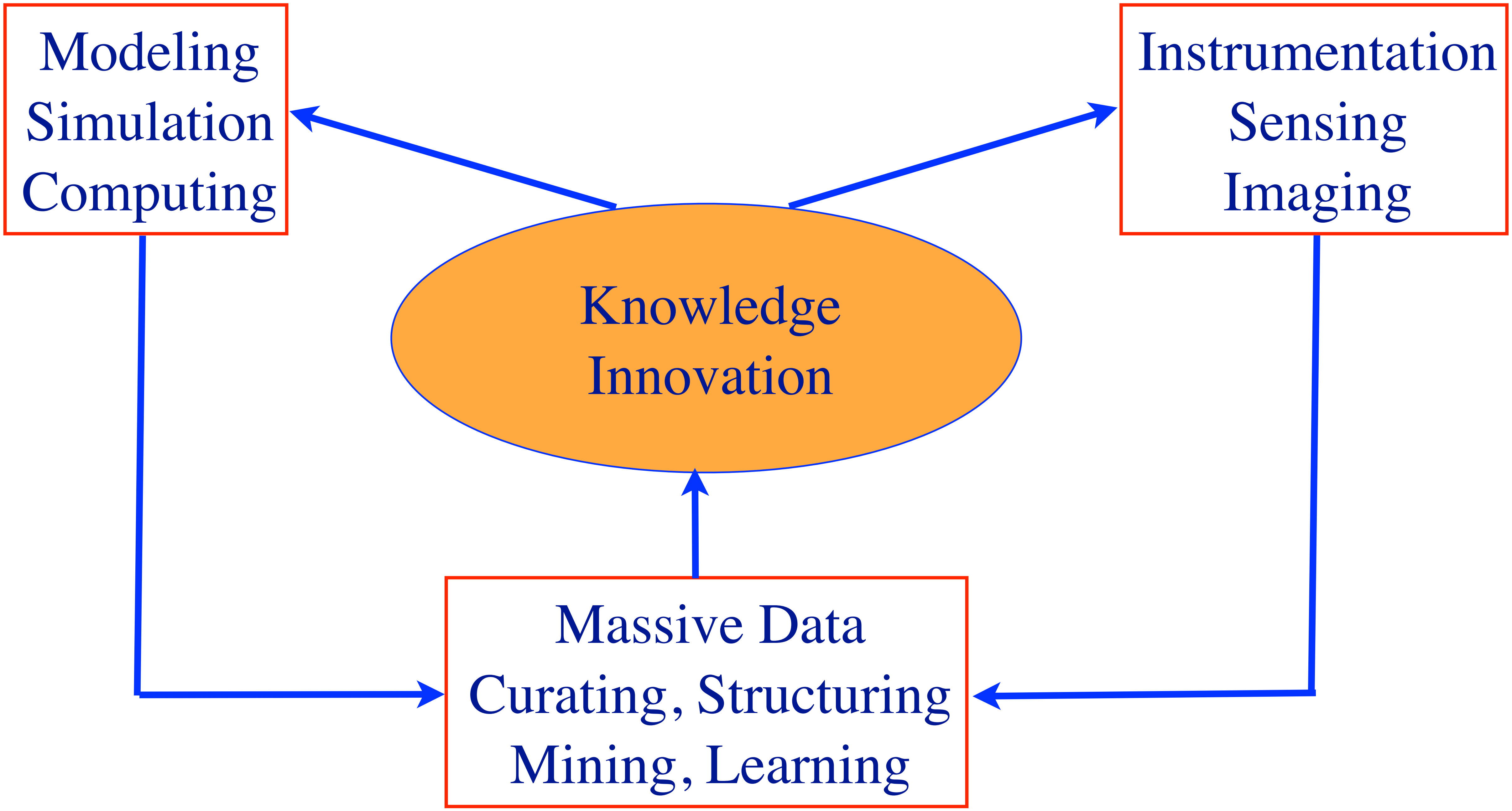
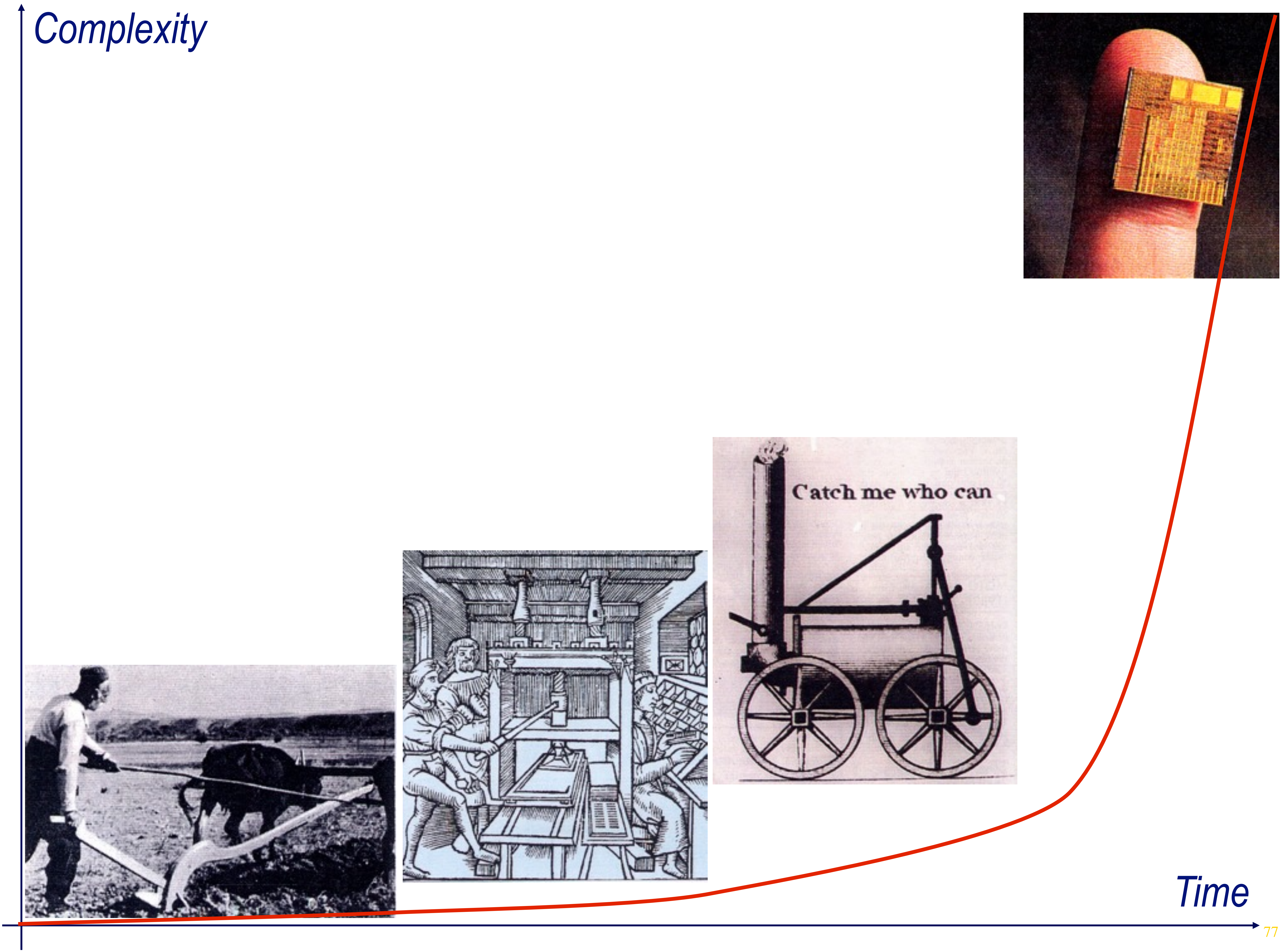
- ✓ Ingredients
- ✓ Impacts
- ▶ Conclusion


Modeling
Simulation
Computing
Instrumentation
Sensing
Imaging
Knowledge
Innovation
Massive Data
Curating, Structuring
Mining, Learning


Complexity
Catch me who can
Time

Conclusion

- CSE
  - Radical change in every area of Science and Engineering
  - Wide access to data and knowledge
  - Critical in addressing human and social development

- Informatics in CSE
  - Should be able to play a central role if
  - Heavily involved in interdisciplinary research