FP7 Support Action - European Exascale Software Initiative

DG Information Society and the unit e-Infrastructures

EESI Final Conference

EESI WG3.4: Life Sciences and Health

Modesto Orozco, Chair

Janet Thornton, Vice Chair

Ramon Goni, speaker

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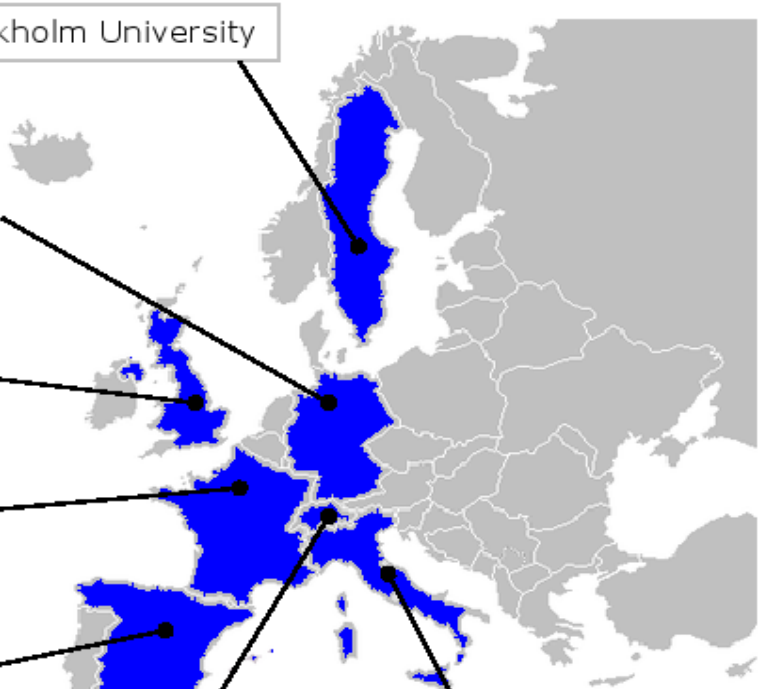
The conclusions of the Life Science panel

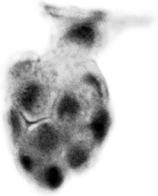


Erik Lindahl	Stockholm University
Helmut Grubmuller	Max Planck Institute
Paolo Carloni	German Research School
Wofgang Wenzel	Karlsruhe Institute of Technology
Reinhard Schneider	EMBL
Janet Thorton/Andrew Lyall	EMBL-EBI
Charles Laughton	University of Nottingham
Richard Lavery	University of Nottingham
Nicolas Baurin	Sanofi-Aventis
Modesto Orozco	BSC
Alfonso Valencia	CNIO
Henry Markram/Felix Schuermann	EPFL
Manuel Peitsch	Swiss Institute of Bioinformatics
Julian.Tirado-Rives (US)	University of Yale
Adrian E. Roitberg (US)	University of Florida
Anna Tramontano	University of Roma

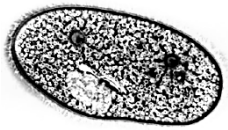
Life Sciences and Health

Population

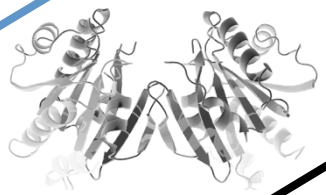
Organ



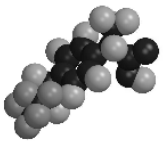
Tissue



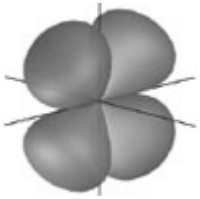
Cell



Macromolecule



Small Molecule



Atom

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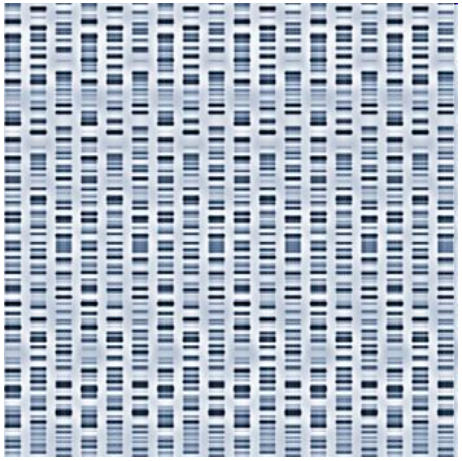
2011 a unique opportunity

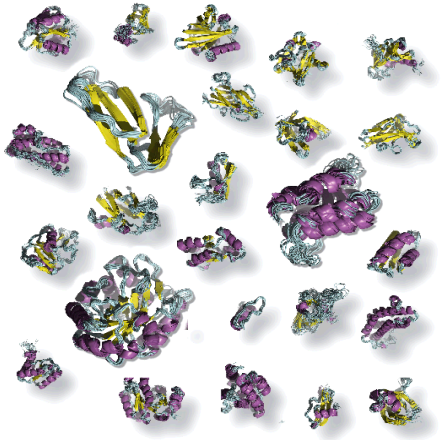


Genomes

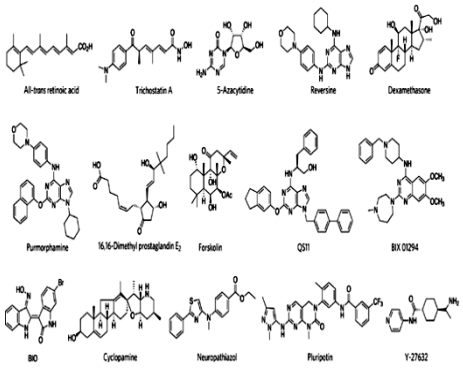
Integration!

Data

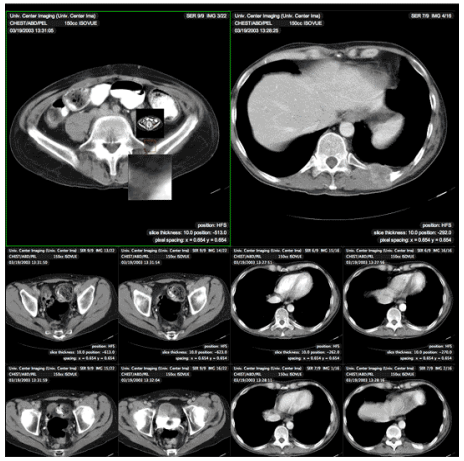
Flops



Structures



Molecules



Images

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human genome project - Buscar con Google - Windows Internet Explorer

http://www.google.es/search?q=human+genome+project&um=1&hl=es&biw=984&bih=548&sou

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Google human genome project

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project is; its progress, history, and goals; what issues are as

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Blog Cite

Human Genome's Breaking Points: Genetic Sequence of Large-Scale Differences Between Human Genomes

ScienceDaily (Feb. 2, 2011) — A detailed analysis of data from 185 human genomes sequenced in the course of the 1000 Genomes Project, by scientists at the European Molecular Biology Laboratory (EMBL)

enlarge

Chinese bioscience: The sequence factory : Nature News - Windows Internet Explorer

http://www.nature.com/news/2010/100303/full/464022a.html

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Published online 3 March 2010 | *Nature* **464**, 22-24 (2010) | doi:10.1038/464022a

News Feature

Chinese bioscience: The sequence factory

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- Genetics
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Stories by keywords
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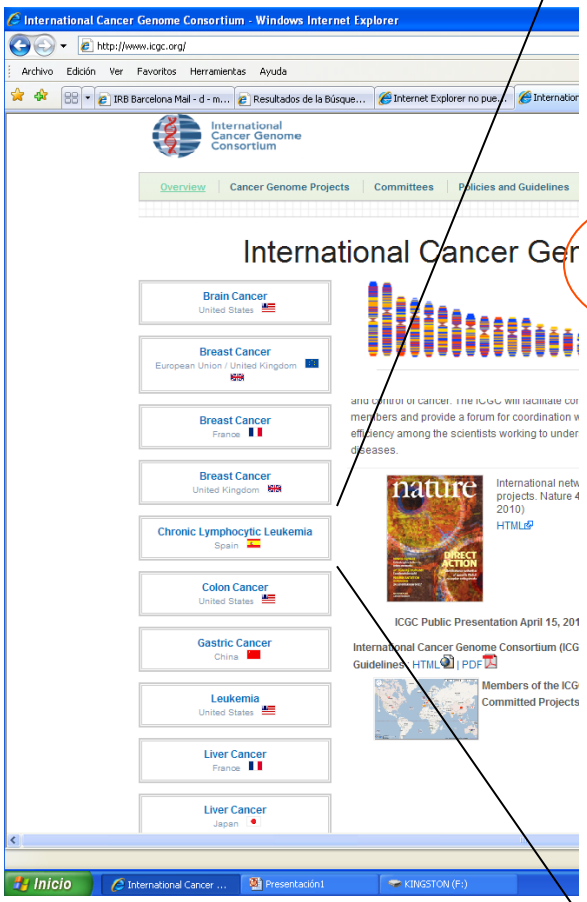
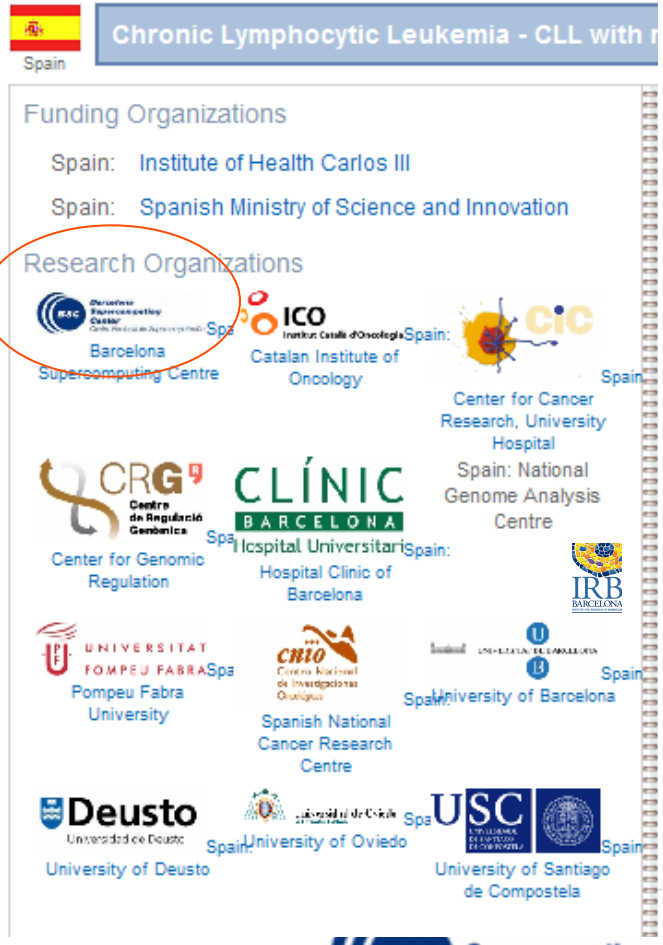
the tally indicates that at least
human genomes will have bee
completed by the end of this n
and that the total will rise to m
than 30,000 by the end of 201

Sequencing the genome of one million citizenships from China

Internation Cancer Genome Project

Experimental data 1 patient < 1 day
Primary analysis 1 patient → 5 days!
Secondary analysis 1 patient → months!





50 cancers

25000 cancer genomes

Puente et al., Nature 2011

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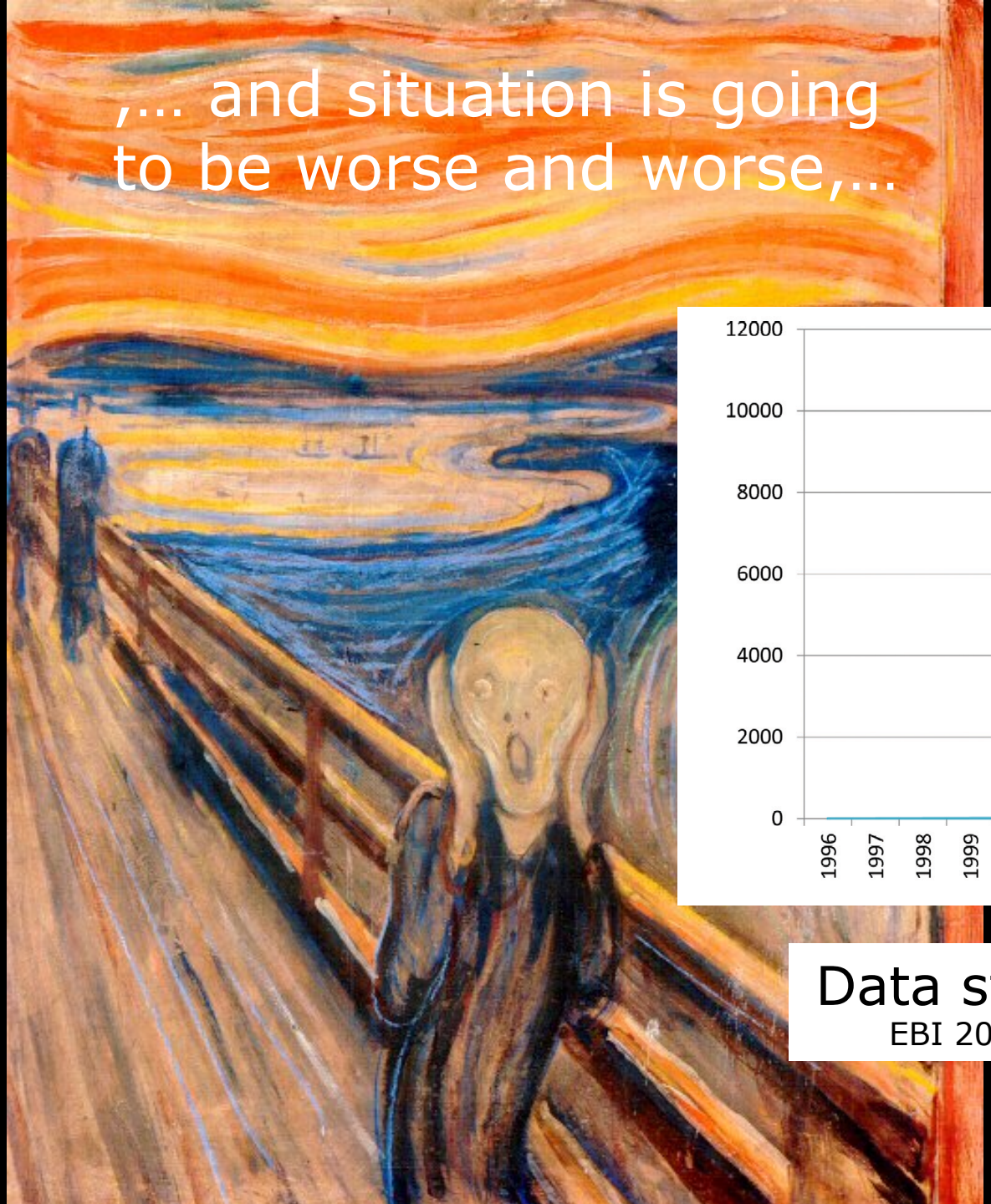
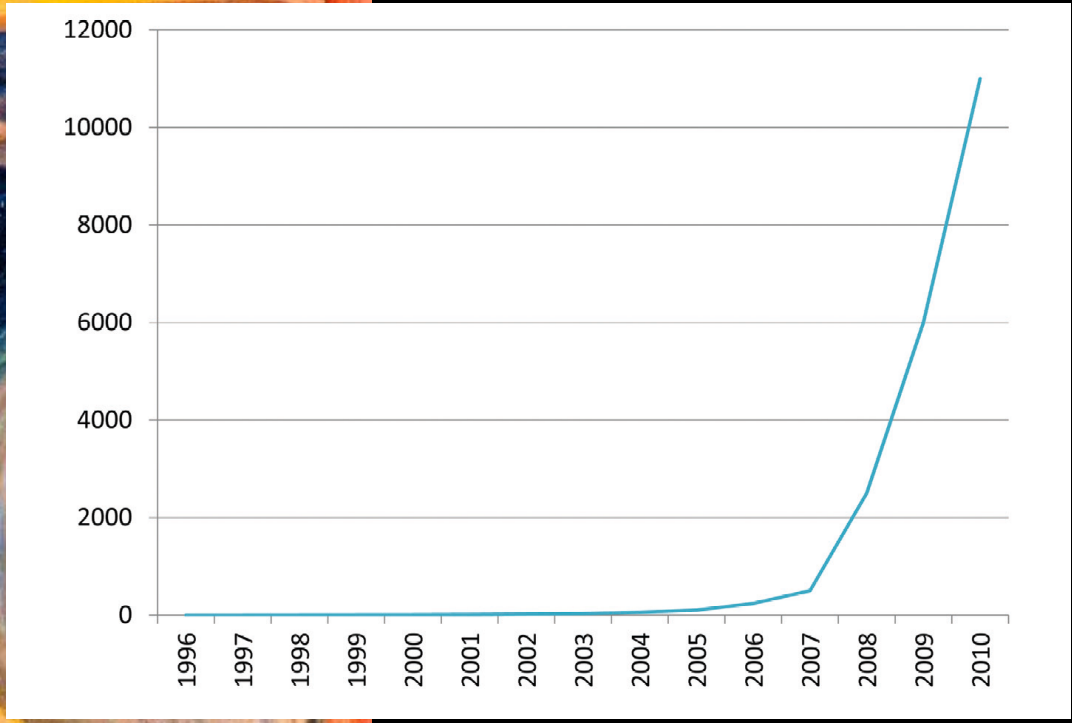
What does it mean,…?

- In BSC experience CLL project:1.5 Pb clean data.
  - We have only 500 patients
  - Analysis means to cross with genomic data for thousands of controls!
  - Data must be confidential, no solutions out of HPC
- CLL implies a sustained use of largest BSC super-computer.
- Computers are becoming the rate-limiting step.



,… and situation is going to be worse and worse,…

ELIXIR

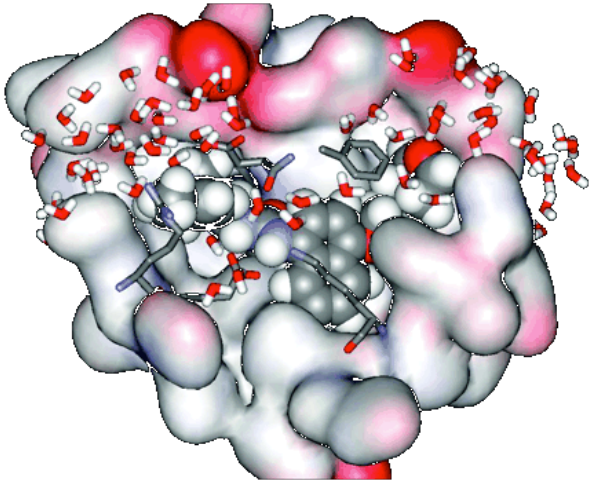


Data storage at EBI (Tb)

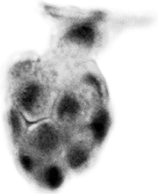
EBI 2010 annual scientific report

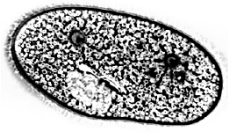
Our dream: simulating life,…

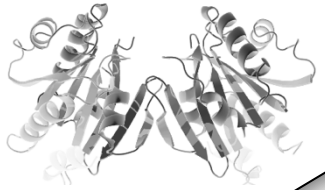
Tremendous impact in reducing the 1.2 Billion $[1] cost of generating a new drug

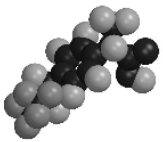


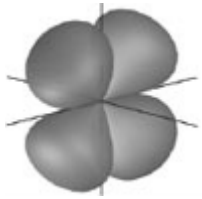
Rational Drug Design











Around 10^5 targets
More than 10^7 drugs
More accurate models!

[1]TUFTS University CSDD Outlook 2008

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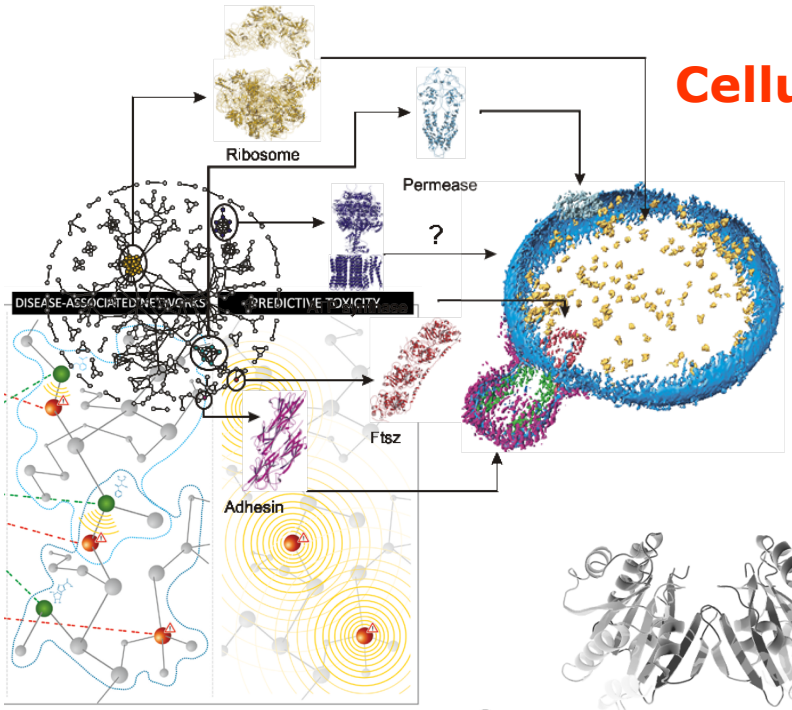
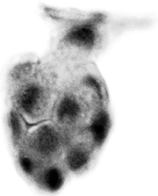
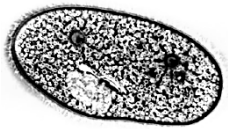
Our dream: simulating life,…

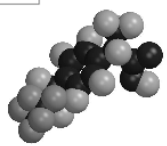
Discovery of new drugs and targets
Reduce side effects and toxicity

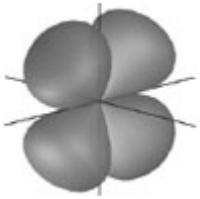


Cellular and subcellular simulation









Integration of different data
Need to define models
CPU might be a major issue

Each cell has 10^9 macromolecules

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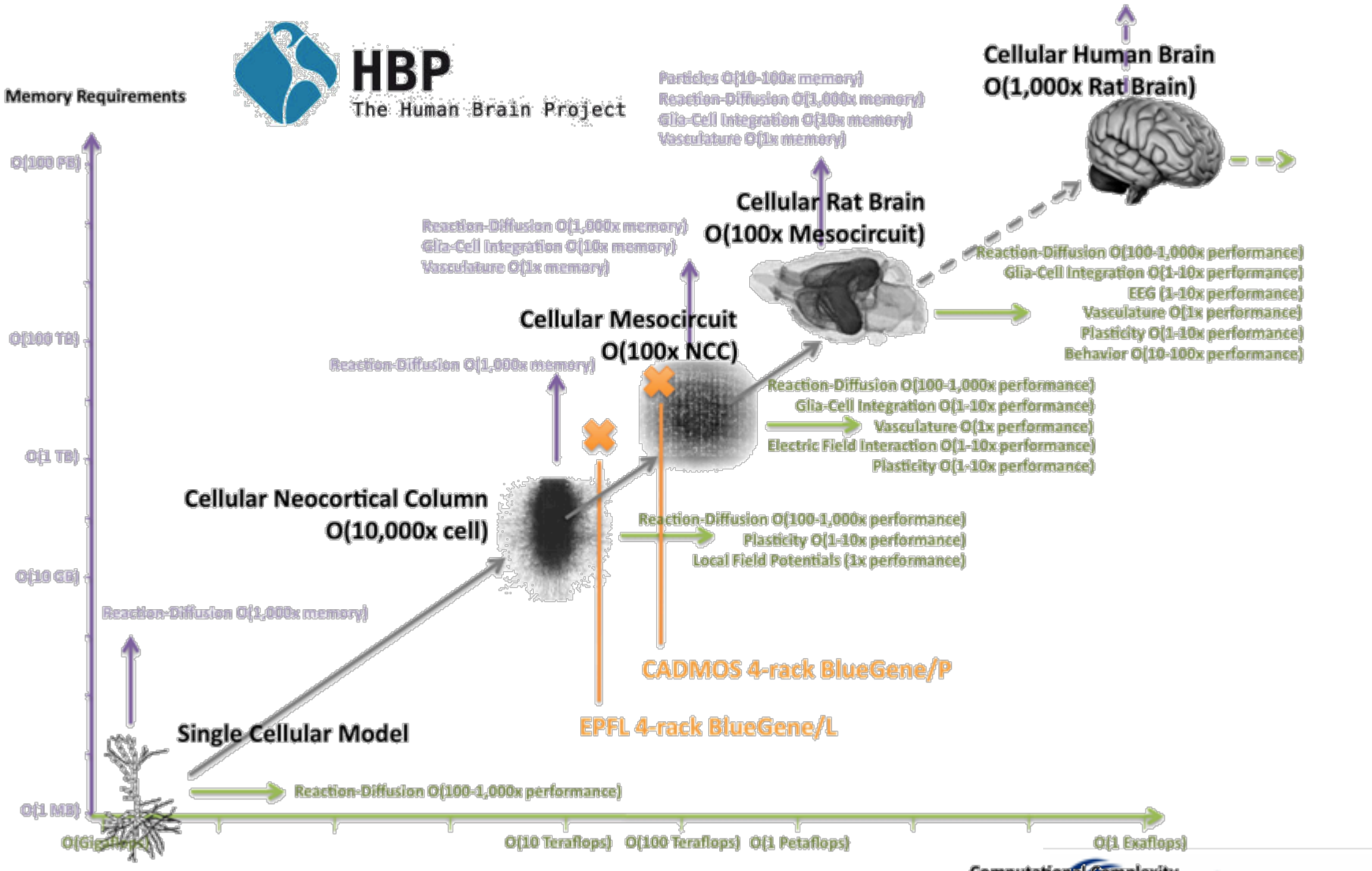
FET: Human Brain Project



F Schürmann, H Markram (Blue Brain Project, EPFL)

Genomics and Personalized Medicine

Data is the main problem

ITFoM

FUTURE OF MEDICINE

Treat patients NOT pathologies

Estimated market 450B$ in 2015[1]

[1]2009 PricewaterhouseCoopers

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Ambition: reinforce Europe position

STRENGTHS

- ELIXIR, Bioinformatics community
- EMBL-EBI
- Research consortia: ENCODE, ICGC, iHEC
- FET Flagships: Personalized Medicine, Human Brain Project.
- PRACE
- Pharmaceutical Industry
- Computational Biology and Bioinformatics Software

WEAKNESSES

- Competitors with privileged access to specialized resources
- No coherent unified data layer available for Bio-data.
- Crucial databases outside Europe.
- Bio-HT techniques are not EU
- Bio-community separated from HPC community

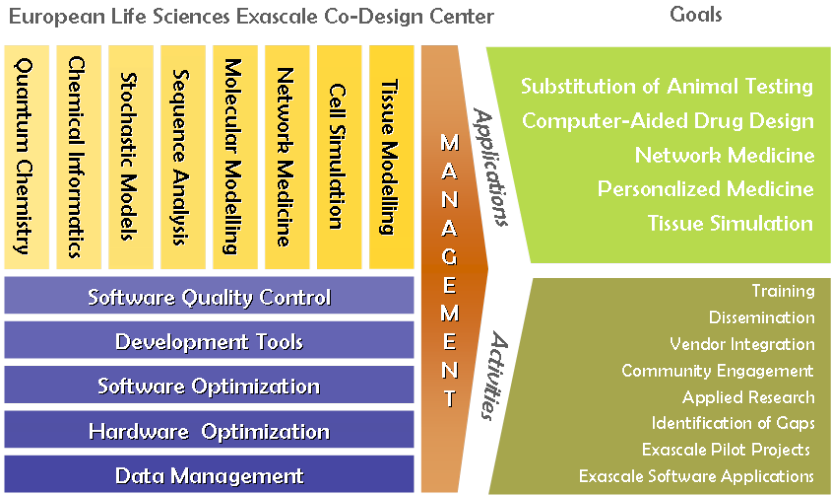
Life-Science needs Exascale

Main conclusions of the panel

- Life science requirements for HPC are enormous and grow exponentially. There is not question that Life Sciences community has ExaScale needs.
- Lack of HPC resources will simply kill several of the most important projects in Life Sciences, including several EU Flagship ones (Human Brain, Personalized Medicine).
- Many other issues rather than FLOPS are important in Life Sciences, often more important.
- **Exascale** should be the keyword, not ExaFlop.
- The experts propose Co-development programs to deploy Exascale to Life Sciences

The Cost

- Estimated around 200 biologists and computer scientist
- Expected investment around 200 MEuros in 2012-2021



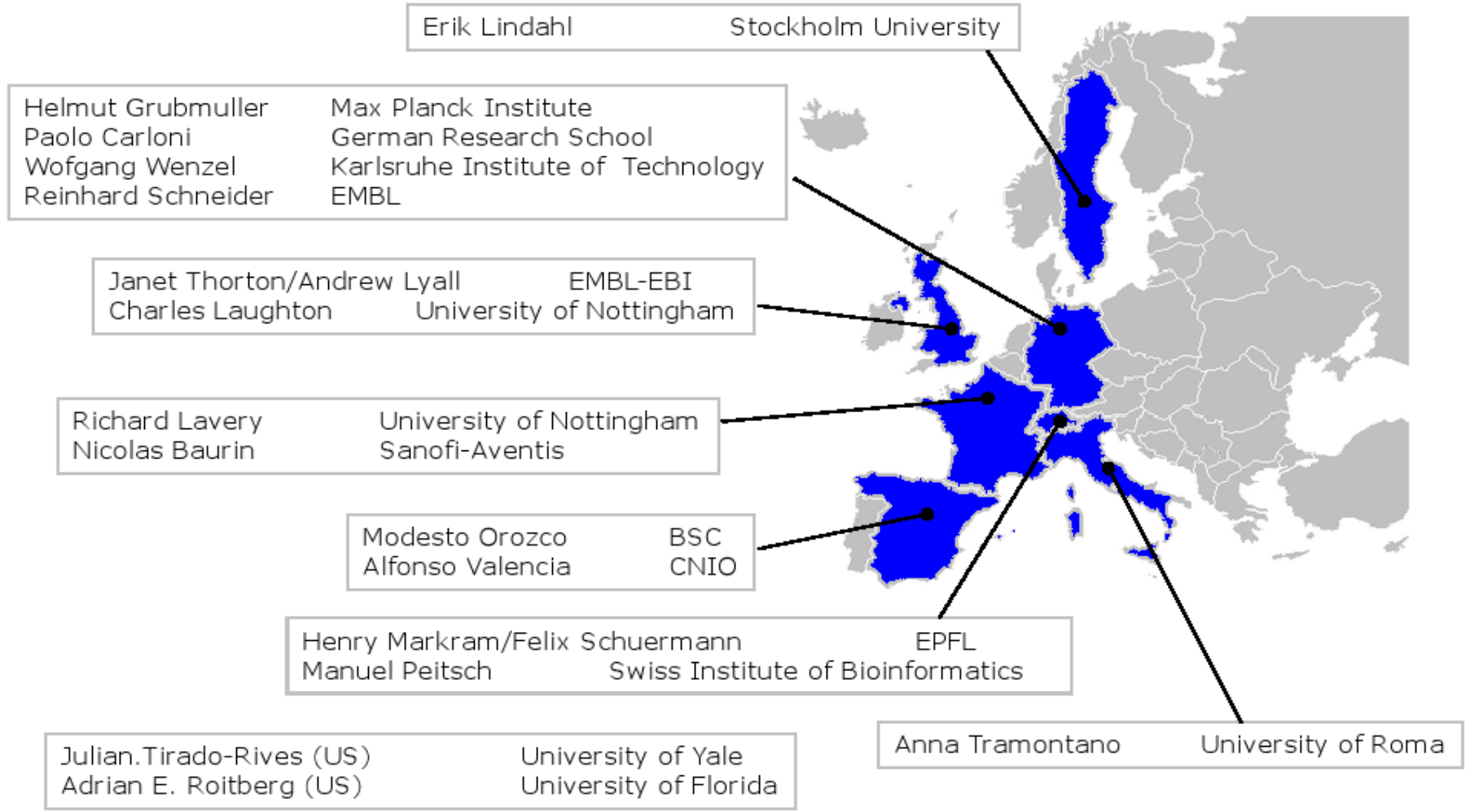
- Public expenditure on healthcare in the EU is around 1,000 B€, the 10% of the GDP.
- The pharmaceutical sector represented a market of roughly 800B€ in 2010
- Europe launches almost the 40% of the pharmaceutical products on the market.
- There are more than 2,100 biotechnology companies in Europe.
- Related areas: cosmetics, food, Environment, Bio-fuels (40% EC Cooperation research budget) will also largely benefit from the initiative.

Impact in health is the crucial issue

One exemple,…

54 million vertebrate animal testing is required to evaluate the safety of major chemicals sold in Europe (see European REACH) Its estimated cost is between 1.3 to 9.5 B€[1].

Animal substitution represents a big reduction of cost of clinical trials by predicting side effect before testing
Development of *in silico* models could simulate entire tissues

[1]http://ec.europa.eu/environment/chemicals/reach/reach_intro.htm

The conclusions of the Life Science panel