



EXCELENCIA

SEVERO

# BSC and HPC Solutions for companies

**Technology Transfer Office** 

## HPC and industrial sector

Many organizations are now using HPC as an essential part of their business strategy. HPC can help them **design new products**, **optimize manufacturing** and delivery processes, solve production problems, mine data, and **Simulate processes**, all in an effort to become more competitive, profitable and "green".

This is done by applying compute cycles in order to **solve problems** in the fastest way possible:

A problem that would take days to solve on a laptop can be solved on a SUPERCOMPUTER in a few minutes





## **HPC:** An enabler for all economic sectors

Materials,
Chemistry &
Engineering

Computeraided Engineering

**Big Data** 

Bio Sciences & Medicine

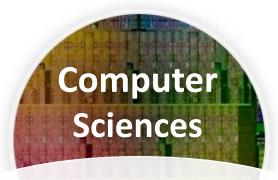
#### **Advances leading to:**

- Improved Healthcare
- Superior Materials
- More Competitive Industry
- Big data an data analytics
- Better Climate Forecasting

Earth and Geo-Engineering



## Mission of BSC Scientific Departments



To influence the way machines are built, programmed and used: programming models, performance tools, Big Data, computer architecture, energy efficiency



To understand living organisms by means of theoretical and computational methods (molecular modeling, genomics, proteomics)



To develop and implement global and regional state-of-the-art models for short-term air quality forecast and long-term climate applications



To develop scientific and engineering software to efficiently exploit super-computing capabilities (biomedical, geophysics, atmospheric, energy, social and economic simulations)



## **Computer Sciences**



**Holistic Computer Architecture Research** 

20 years innovating in **Programming Models** 

Performance Analytics
Tools: From Data to Insight

Race towards Exascale

HPC and Big Data convergence

Artificial Intelligence era

Multiple architectures for different applications domains



## **Earth Sciences**

Environmental modelling and forecasting, with a particular focus on weather, climate and air quality

Modeling
air quality and
Sand and Dust Storms
Processes from urban to
Global and the impacts
on weather, health
and ecosystems



Climate
predictions
system from
subseasonal-to-decadal
forecasts

#### **Service Users Sectors**



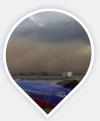
Infrastructures



Solar Energy



Urban development



Transport



Wind Energy



Agriculture



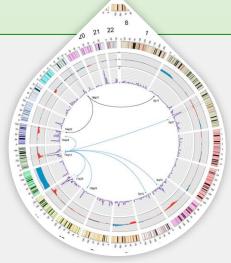
Insurance



## Life Sciences

## Computational Genomics

Design, development, and use of bioinformatic protocols and tools in the context of comparative genomics and analyses of gene and protein collections.



# Protein modelling and drug discovery

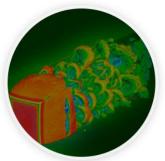
Theoretical and computational approaches to protein interactions, and study of complex biochemical processes at electronic and atomic theoretical detail.

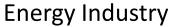




## **CASE**

Our mission is to develop computational tools to simulate highly complex problems and that exploit efficiently the supercomputing capabilities





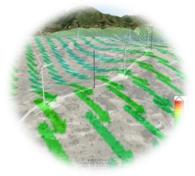
Aeronautic and automotive Industry
Aerodynamics
ATM in dust conditions
Composite materials



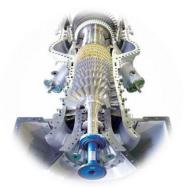
Innovative Manufacturing
Biomechanics (cardiovascular system,
respiratory system)
Smart Cities

Agent-based models











## BSC TECHNOLOGICAL PORTFOLIO



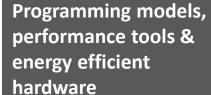
**Pharma** 



Medical



**Bioinformatic tools** for target and drug discovery



**Embedded electronics** 

for improving safety in

time-critical applications



Mobile



**HPC** 





**Smart cities** 



**Big Data** 



Weather / **Climate Agencies** 



Renewables



**Agriculture** 



Air quality, weather and climate modelling products

Simulations of complex problems



Middleware, **System Software** 



**HPC** 



**Smart Cities** 



IoT



Cloud



**Big Data** 







Medical



**Nautical** 



Oil & Gas



**Engineering** 



Automotive



**Smart Cities** 



**Aviation** 



**Automotive** 



Rail



**Aviation** 



**Space** 

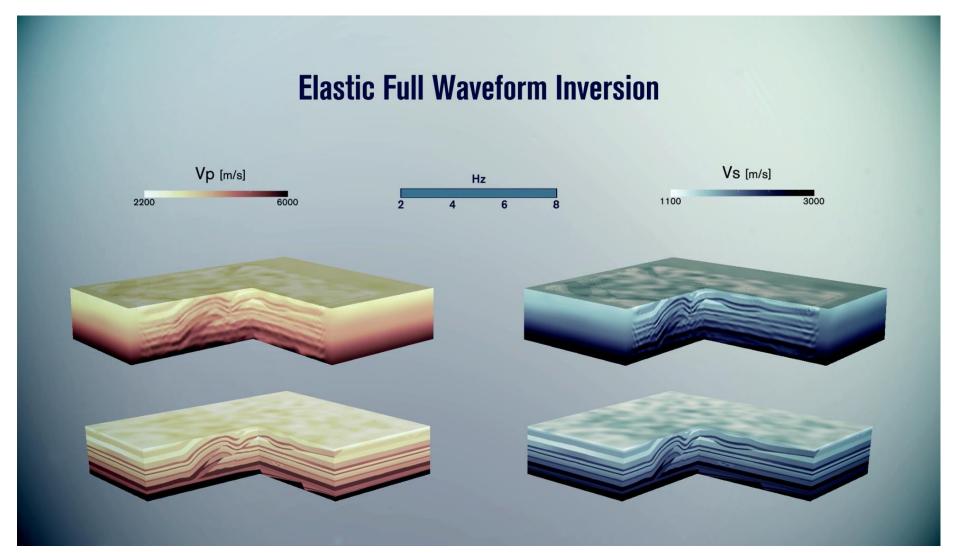


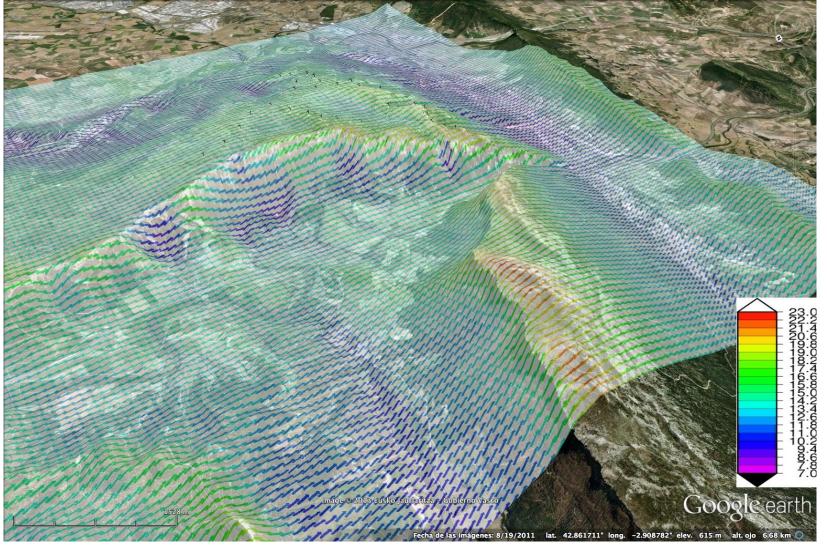
**Pharma** 



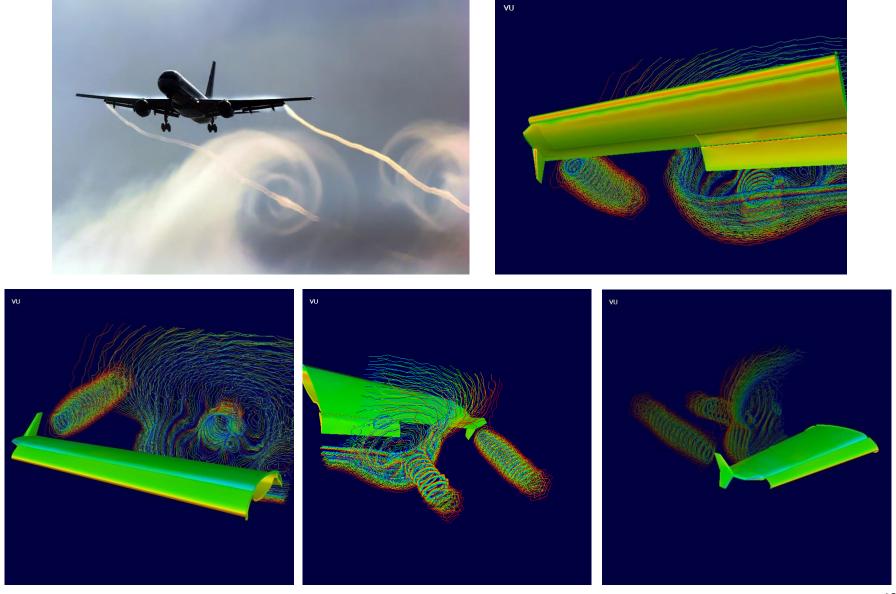


## Energy: REPSOL-BSC Research Center

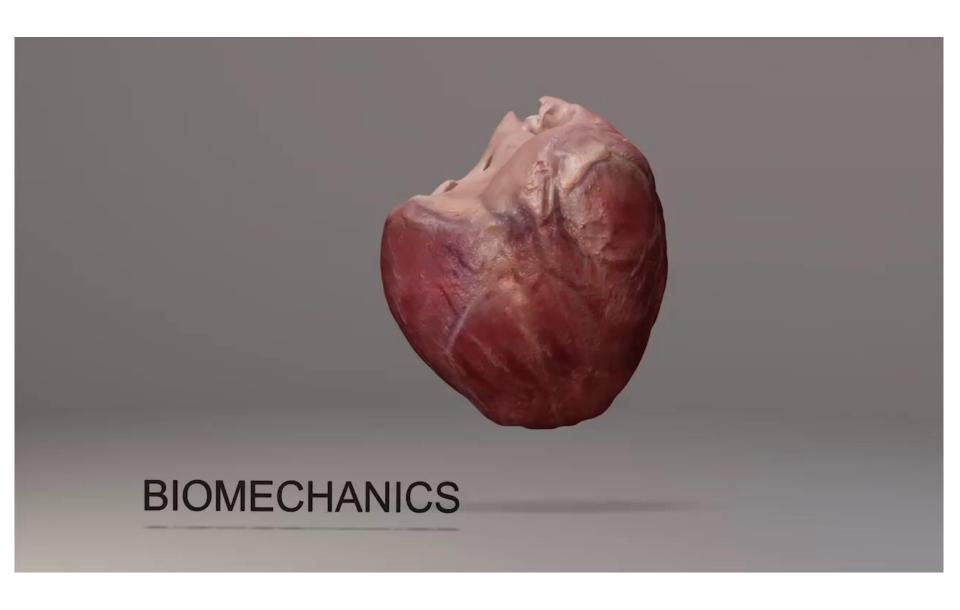


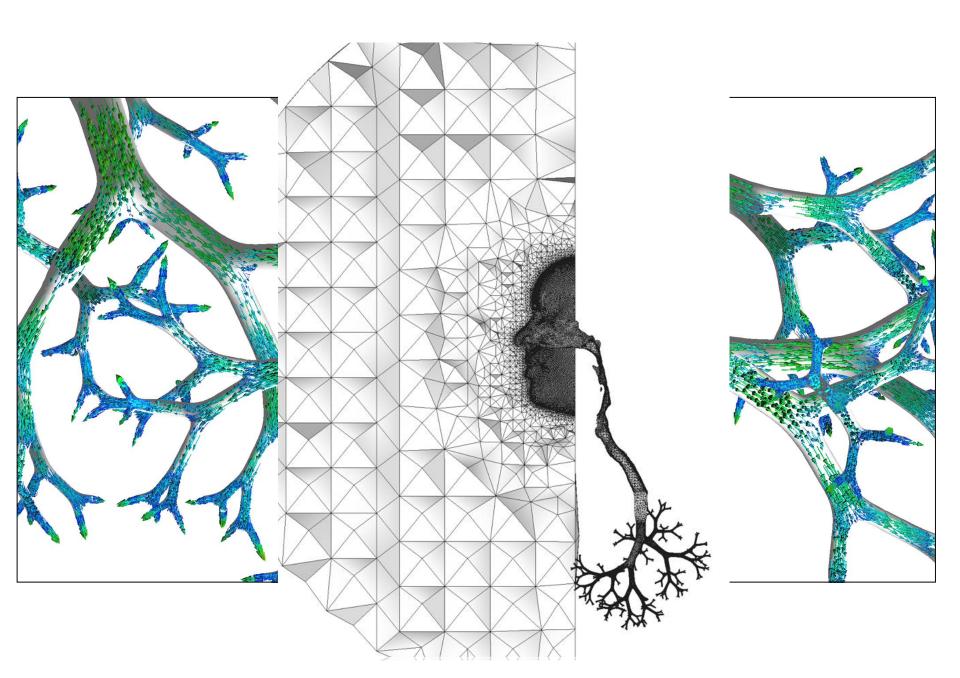












#### **Urban Planning Prototype URBAN MODEL Building project Air Quality Ecological** Exploration and query tool Urbanism Mobility & Public space Waste Submodels **Ontologies** Wat **B**jodiversity Energy Food production **INDICATORS TESTING & ASSESSMENT** Data SCENARIO 1 SCENARIO 2 SCENARIO 3 SCENARIO ... Data **ECOLOGICAL URBANISM CERTIFICATION** B G D B EXCELLENT GOOD SUFFICIENT INSUFFICIENT VERYINSUFFICIENT Data Maximum points: 20 Points attained: 18 LAND OCCUPATION Scored attained: 90% Maximum points: 100 Points attained: 81 Scored attained: 81% Maximum points: 70 Points attained: 44.6 Theme weight: 25% % attained: 18,9% (out of 25%) 143.6 points out of 190 Scored attained: 63,7% Final rating: **URBAN COMPLEXITY URBAN COMPLEXITY** Maximum points: 50 Points attained: 37,5 Scored attained: **75%** 74.7% Maximum points: 40 Points attained: 32 Scored attained: **80%** GREEN SPACES AND BIODIVERSITY METABOLIC EFFICIENCY Maximum points: 130 Points attained: 94,4 Scored attained: **72,6% URBAN METABOLISM** grocery store hotel industrial institutiona parking Points attained: 44 Scored attained: 73,3% GOOD restaurani retail vacant Agència **ECOLOGIA** d'Ecologia Urbana

de Barcelona

## Joint Research Centers (JRC)











## Multi Annual Framework Agreement (MAFA)









## **Customized R&D Projects**







### **Industrial PhD**







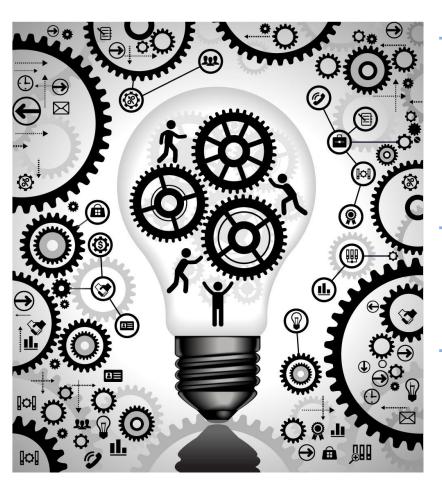






**European Space Agency** 

## **How to Collaborate**



- Customised R&D projects with companies
  - Joint Research Centers
  - Multi-Annual Framework Agreement
  - Customized R&D projects
  - Industrial PhD
- Accessing BSC technologies through licenses
  - To our Patent Portfolio
  - To our Software Portfolio
- Service Platform
  - Pay per Service (computational genomics, air quality, big data)
  - Software as a Service



## **Success stories**

Climate projection for a Spanish wine Company by Earth Sciences Services



After request of a winemaker interested in identifying potential sites for grape plantation in the South America, we performed an analysis to identify if and where it will be possible to grow grapes in 2050. Six wine indices accounting for climate projections of temperature and precipitation were used in the assessment.

#### Partners and collaborators























#### **Projects**











## First BSC's Spin Off

**Nostrum Biodiscovery: How a drug finds its target** 





## PELE transfered to market



spin-off that applies
supercomputing to speed up drug
discovery (12-07-2016)

Nostrum Biodiscovery aims to help its clients speed up the first stage of drug development

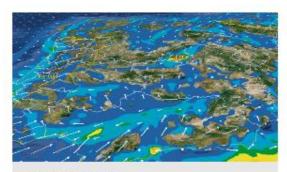
"it is estimated that the approach used by Nostrum BioDiscovery can reduce the early-stage drug development by up to **two years** (the discovery phase prior to pre-clinical trials) and cut costs by 15-20% in this first phase, **implying** an estimated saving on average of 40 million euros."

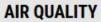
Experience and cutting-edge supercomputational technologies: PELE, ED/MD, MDWeb, MoDEL

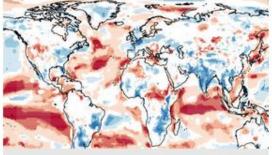




## **Service Platform**



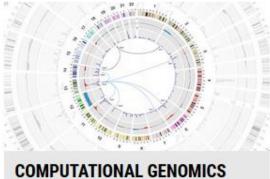




CLIMATE



MINERAL DUST





**HPC PERFORMANCE ANALYSIS** AND OPTIMIZATION







**EXCELENCIA** 

**SEVERO** 

**OCHOA** 

More info. at: www.bsc.es

# Thanks!

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