Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

Life Sciences Dept Barcelona Supercomputing Center

Alfonso Valencia

ICREA Prof

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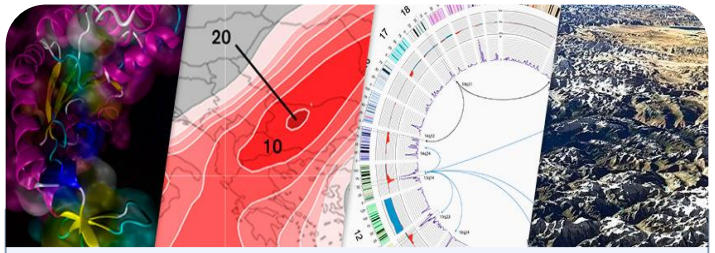
BSC-CNS objectives

Supercomputing services
to Spanish and EU researchers



R&D in Computer, Life, Earth and
Engineering Sciences

PhD programme, technology
transfer, public engagement

BSC-CNS is a consortium that includes

Spanish Government	60%
Catalan Government	30%
Univ. Politècnica de Catalunya (UPC)	10%

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MareNostrum 4

Total peak performance: **13,9** Pflops

General Purpose Cluster:	11.15 Pflops	(1.07.2017)
CTE1-P9+Volta:	1.57 Pflops	(1.03.2018)
CTE2-Arm V8:	0.65 Pflops	(12.2019)
CTE3-AMD:	0.52 Pflops	(12.2019)

PRACE

Access: prace-ri.eu/hpc_acces

RES
RED ESPAÑOLA DE SUPERCOMPUTACIÓN

Access: bsc.es/res-intranet

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MareNostrum 1
2004 – 42,3 Tflops
1st Europe / 4th World
New technologies

MareNostrum 2
2006 – 94,2 Tflops
1st Europe / 5th World
New technologies

MareNostrum 3
2012 – 1,1 Pflops
12th Europe / 36th World

MareNostrum 4
2017 – 11,1 Pflops
2nd Europe / 13th World
New technologies

Recursos disponibles

MareNostrum 4
2017-2022

Storage disco
15 PB

11.1 PFlops, propósito General (x86)
1,6 PFlops, aceleración **con GPUs**
0,65 PFlops CTE-ARM
0,5 PFlops CTE-AMD GPUs

Storage
en cintas
150 PB

MareNostrum 5
2022-2027

> 200 PFlops , incluyendo Propósito General y aceleración **con GPUs y Clusters de arquitecturas emergentes/disruptivas**

Storage disco
+150 PB

Storage
en cintas
+400 PB

740 scientist and engineers

Largest Research Institute in Spain

100 M € from H2020

The third Spanish Institution in EU funding

4 Departments

Earth, Engineering, Computer Science & Life

Life

6 Research Group + 5 support Units

130 scientist

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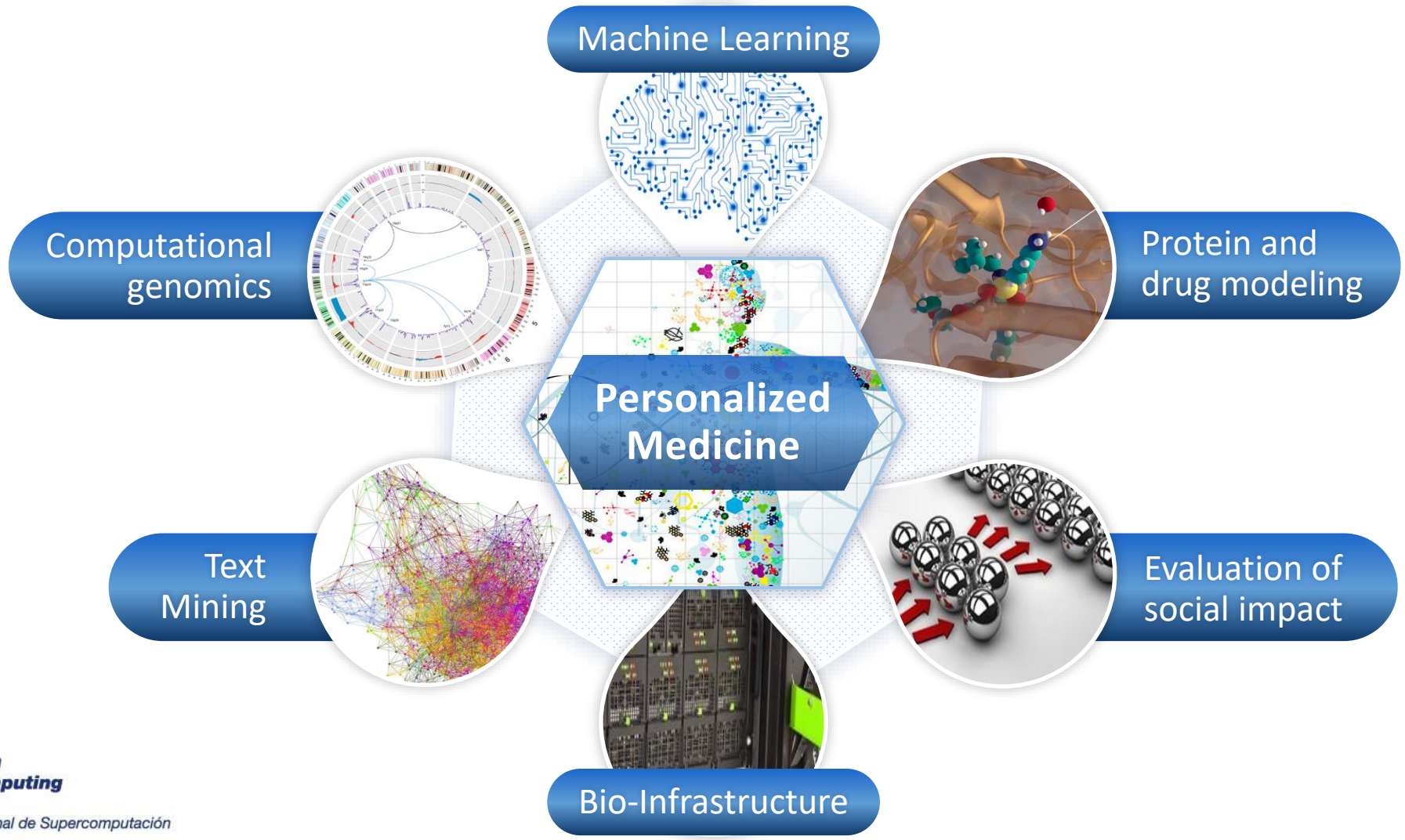
Life Sciences

Understanding living organisms by theoretical and computational methods



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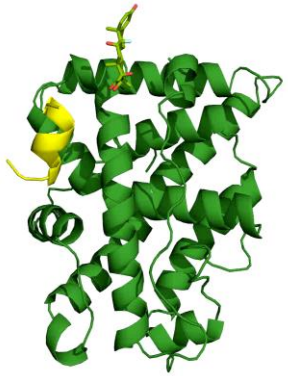
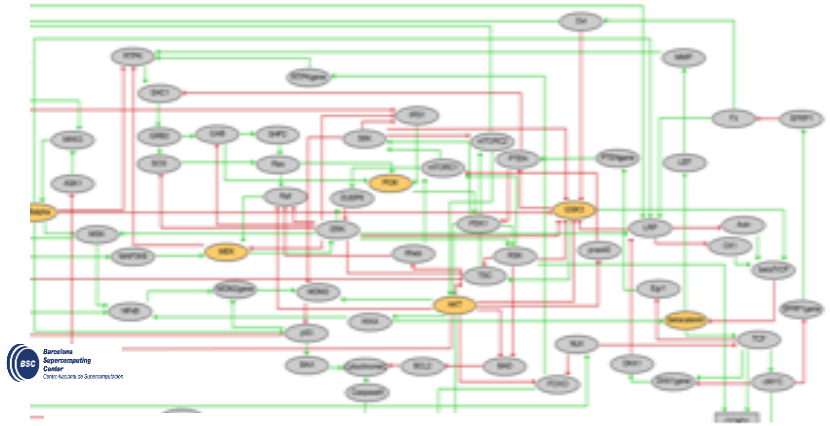
Simulations from molecules, to cells, to organs …

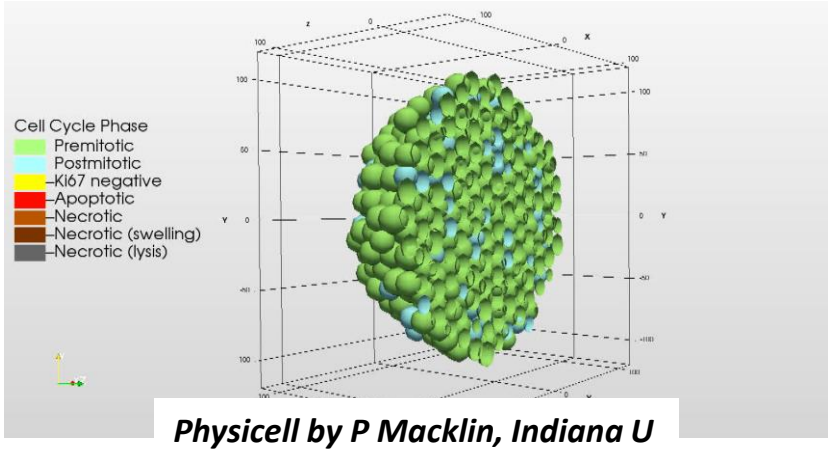


By Victor Guallar ICREA & BSC

By Mariano Vazquez, CASE - BSC



MABOSS Cell Modellng Framework



Physicell by P Macklin, Indiana U

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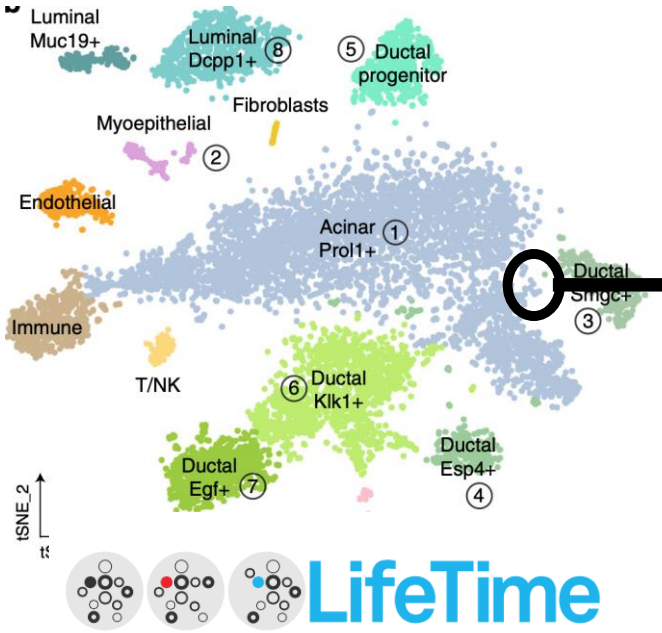
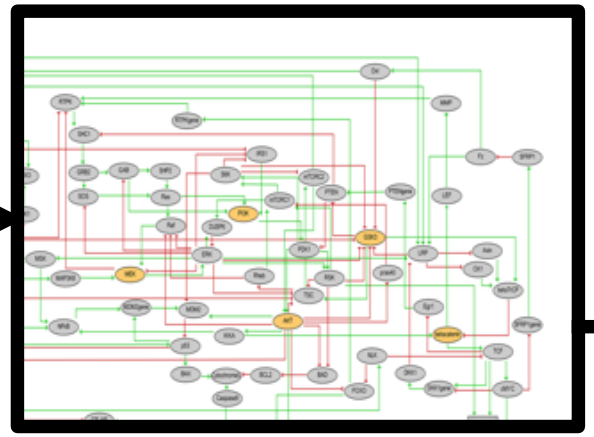
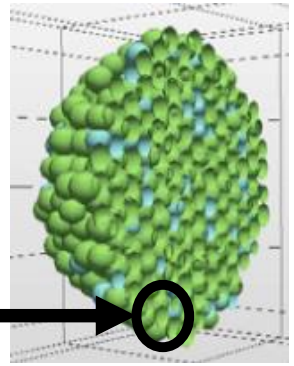
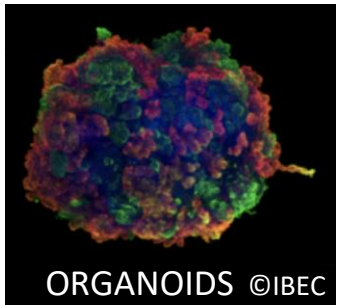
From Single Cell Data to Models

HPC/Exascale Centre of Excellence in Personalised Medicine









End Users Communities

*”Replace the current generation of bioinformatics methods with **cellular models, providing mechanistic descriptions and testable hypotheses**, instead of current statistical approximations and intuitive descriptions”*

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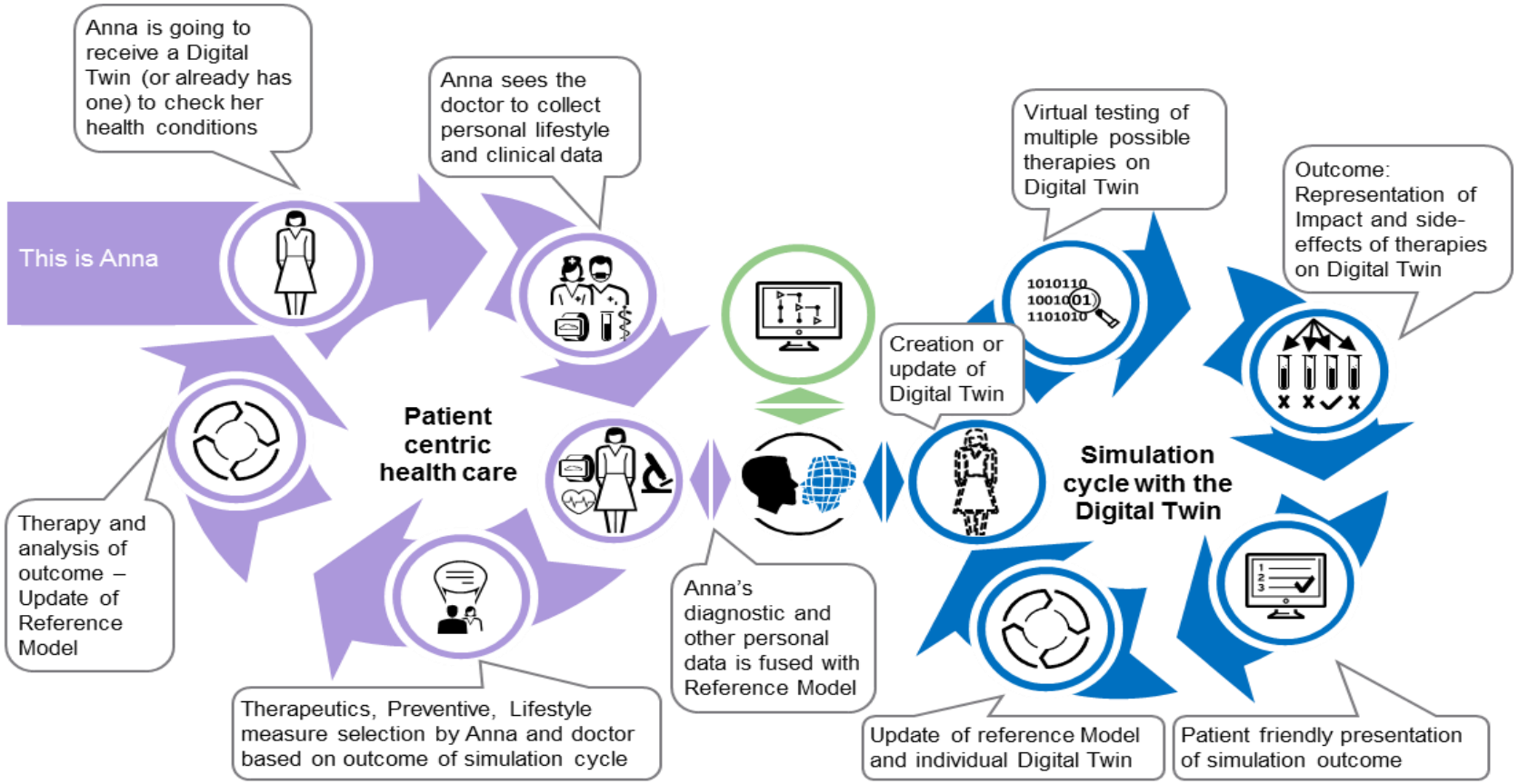
Digital Twin for Future Medicine



Is this scenario possible?
When will it be possible?
To what level?
For what medical problems?

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Life Sciences 2021

Life Sciences

Genomic Regulation *JRG*

Investigación Programa Ramón y Cajal

Computational Genomics

ICREA

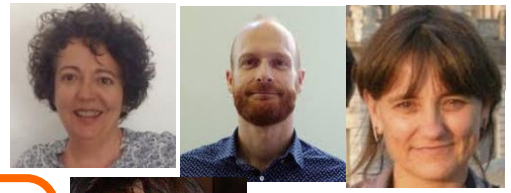
Microbial Genomics

IRB Barcelona · erc · ICREA

Genome Informatics

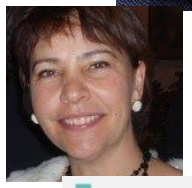
NTNU

Text Mining



Plan TL — Plan de Impulso de las Tecnologías del Lenguaje

Social Impact



bioinfo4women

Biological Networks

erc · ICREA

Computational Biology

ICREA

Protein Modeling

ICREA

Computational Bioinformatics

Universitat de Barcelona

INB ELIXIR-ES

Instituto de Salud Carlos III · INB · IMPaCT · elixir SPAIN

Coordination Node

Barcelona Supercomputing Center — Centro Nacional de Supercomputación

Milana Morgenstern Bar-Ilan

Vera Pancaldi Toulouse

Joaquín Dopazo Seville

Biola Javierre F Carreras

Anïs Baudot U. Marseille

Osnat Hakimi UIC

Eudard Porta F. Carreras

Areas of Interest

Infrastructure (EUCANshare, EnCanImage, **EUCANCan,** EOSC-LIFE, ELIXIR-Converge)

>>> INFRA-2021-EOSC-01-02: FAIR ..COVID-19 and other infectious diseases

>>> INFRA-2021-EOSC-06 -06: FAIR ..Cancer

Network biology/biomedicine (INFORE, AI-SPRINT)

>>>> CL4-2021-HUMAN-01-01:Verifiable robustness, …Trustworthy AI.

>>>> HLTH-2021-CARE-05-02: Data driven decision support…

European Health Data Space (**HealthyCloud,** Patologic, iPC)

>>> HLTH-2021-DISEASE-04-03: Innovative approaches ..diseases .. in sub-Saharan Africa

>>> HLTH-2021-tools-06-03: Innovative tools for use .. of health data (in particular EHR).

>>> new call Cancer Mision.

Protein Engineering (FuturEnzyme, OXIPRO)

>>> future enzyme engineering and modelling

AI/ML

>>> CL4-2021-HUMAN-01-24 Tackling gender, race and other biases in AI (RIA)

>>> HLTH-2022-STAYHLTH-01-04 Trustworthy AI tools to predict … chronic diseases …(RIA)

Modelling HPC (**PerMedCoE**)

>>> **PerMedCoE 2**

>>> Future call in the context of "Digital Twins"

NLP (IntelComp, ELE, MT4ALL, **nextProcurement**)

>>> Connecting Europe Facility (CEF2) , The Digital Europe Programme

Disinformation/Fake news (IBERIFIER)

>> CL4-2021-HUMAN-01-27: AI to fight disinformation (RIA)

MSCA

>>>> **MycoXplore**

Perfil de empresa con las que la entidad estaría interesada en trabajar para presentar proyectos europeos

Others

- En el entorno clínico empresas con sistemas software implantados para gestion de datos, NLP y AI/ML

- Modelado de metabolismo o sistemas similares

- Modelado económico en salud / economia de la salud

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