PerMedCoE

HPC/Exascale
Centre of
Excellence in
Personalised
Medicine

PROJECT OVERVIEW

OVERVIEW

PerMedCoE
Grant agreement ID: 951773

Status
Ongoing project

Start date
1 October 2020

End date
30 September 2023

Funded under
H2020-EU.1.4.1.3.

Overall budget
€ 4 999 567,50

EU contribution
€ 4 999 567,50

Coordinated by
BARCELONA SUPERCOMPUTING CENTER -
CENTRO NACIONAL DE SUPERCOMPUTACION

🇪🇸 Spain

BSC Barcelona Supercomputing Center
Centro Nacional de Supercomputación

PARTNERS

MISSION

PerMedCoE is the HPC/Exascale Centre of Excellence for Personalised Medicine in Europe

Our motivation

The performance of current simulation software is still insufficient to tackle medical problems such as tumour evolution or patient-specific treatments.

Simulation of cellular mechanistic models are essential for the translation of omic data to medical relevant actions and these should be accessible to the end-users in the appropriate environment of the PerMed-specific big confidential data.
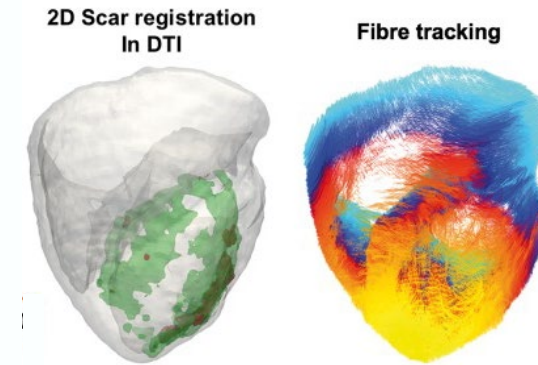
Our vision

The challenge is to develop a sustainable roadmap to scale-up the essential software for the cell-level simulation to the new European HPC/Exascale systems.

Our goal is **to provide an efficient and sustainable entry point to the HPC/Exascale-upgraded methodology** to translate omics analysis into actionable models of cellular functions of medical relevance.
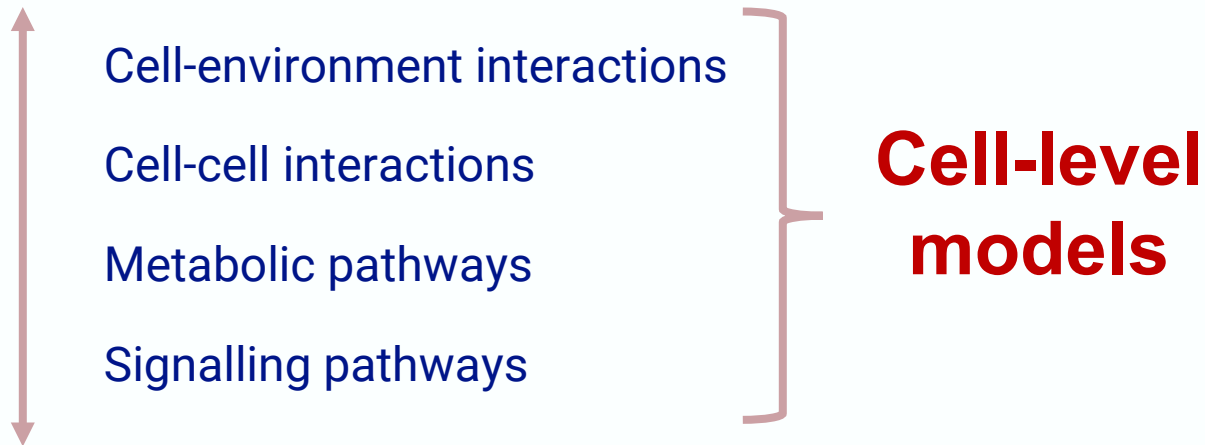
www.permedcoe.eu

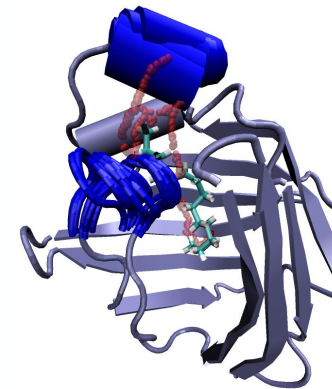# PerMedCoE aims to integrate PerMed into the new European HPC/Exascale ecosystem

2D Scar registration In DTI

Fibre tracking

Europace. 2019 May, 21(5): 822–832.

- Physiological-level models (Fluid dynamics – **CompBioMed**)

Cell-environment interactions

Cell-cell interactions

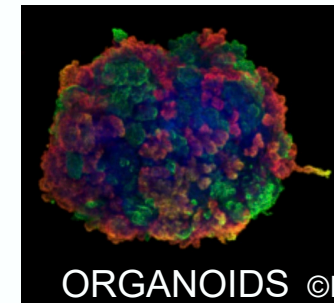**Cell-level models**

Metabolic pathways
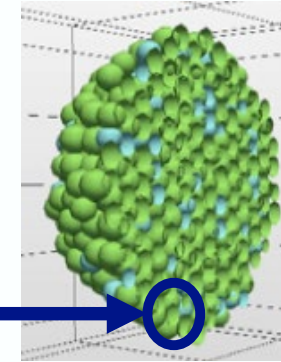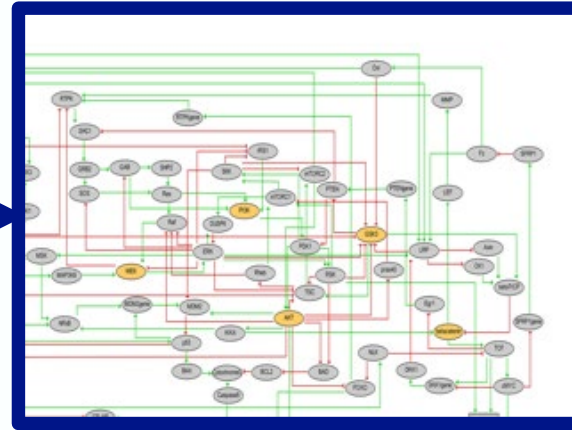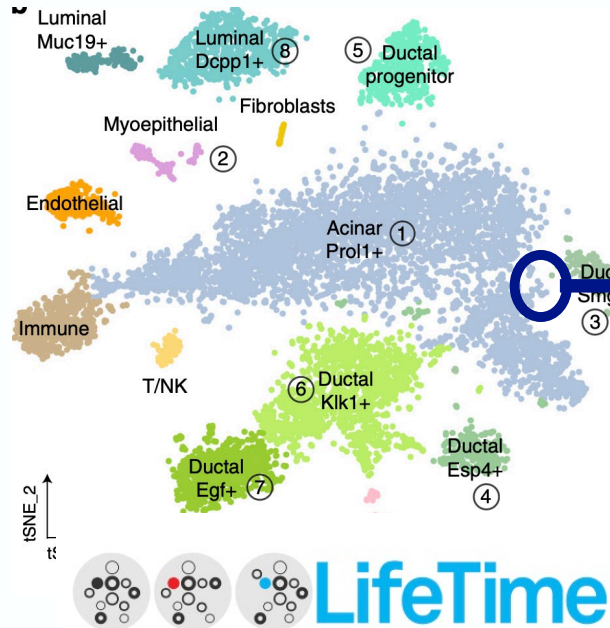
Signalling pathways

- Atomic-level models (Molecular dynamics – **BioExcel**)
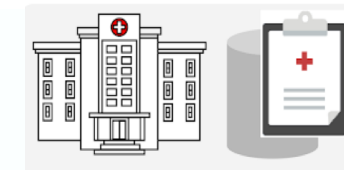

J. Chem. Theo. Comp. 2005, 6, 1304-1311

From Single Cell Data to Models
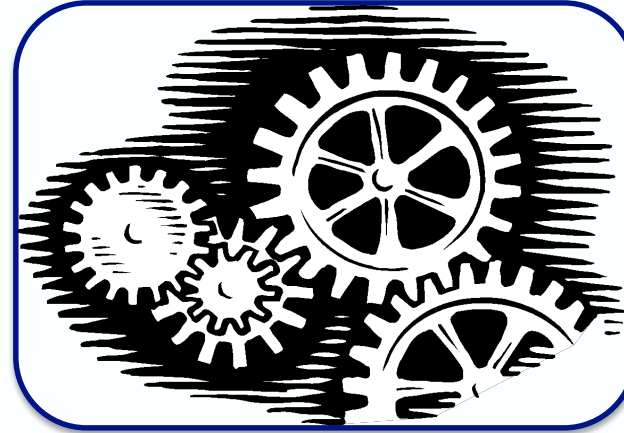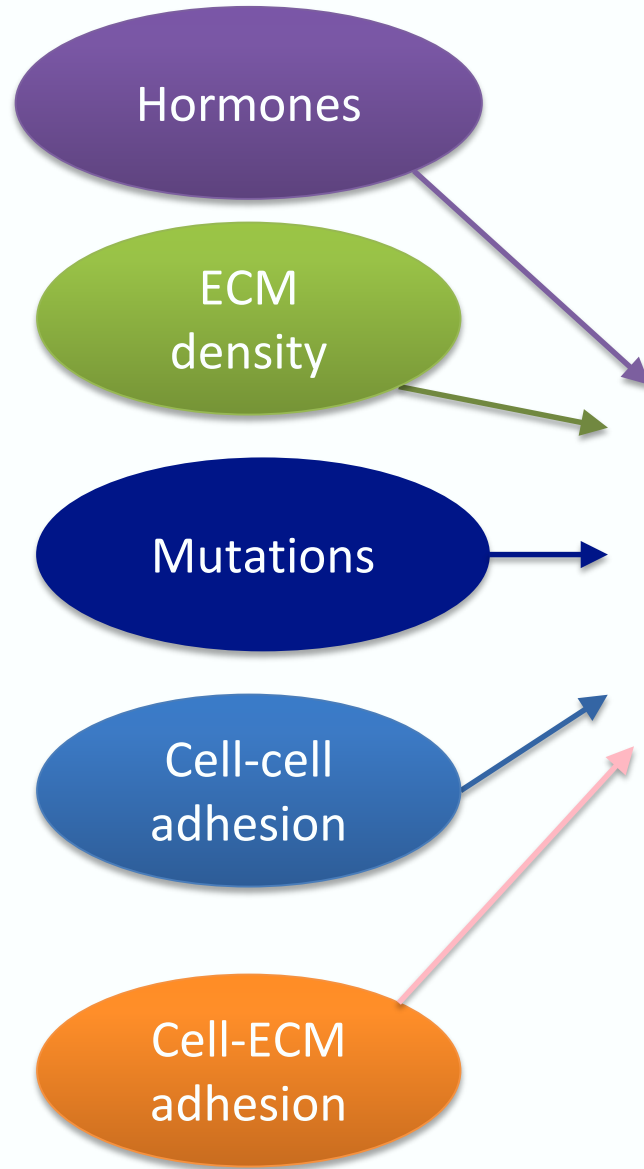

ORGANOIDS ©IB

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"*

# The motivation: Genotype-to-phenotype modelling

Hormones

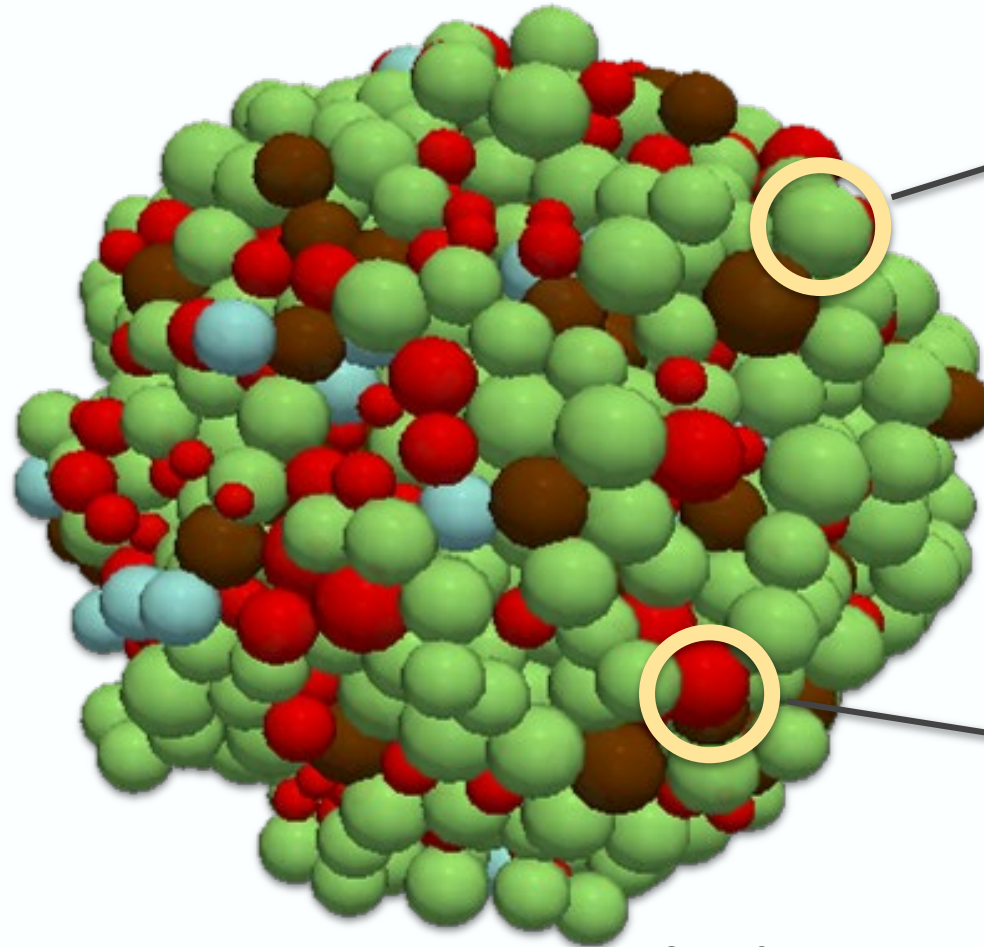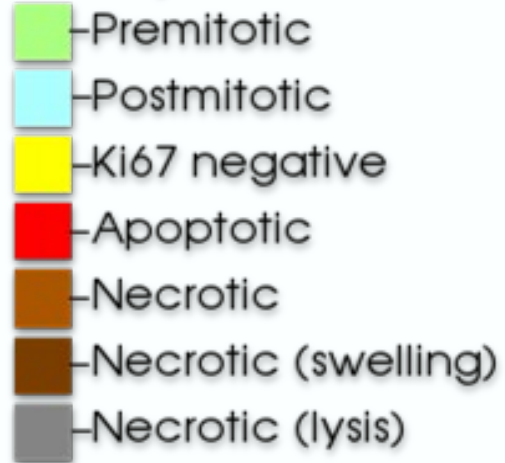ECM density

Mutations

Cell-cell adhesion

Cell-ECM adhesion

Multiscale modelling
Gene mutations
Signalling pathways
Cell - environment
ECM modification

Friedl and Alexander, *Cell*, 2011

Cells have different phenotypes depending on their genes' activation

Different cells have different signalling states

Slide from M. Ponce de León, BSC
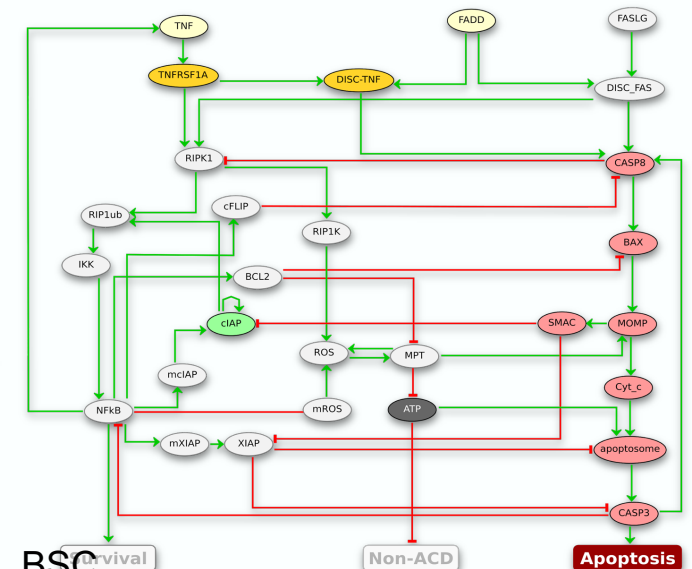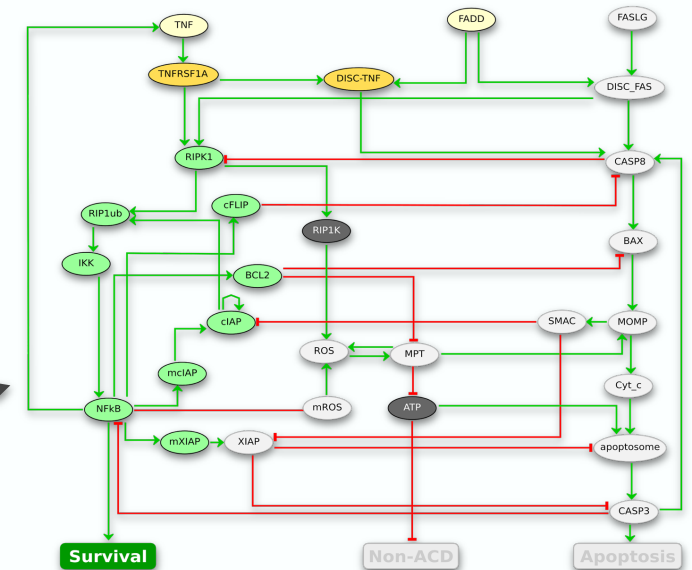
CORE APPLICATIONS

PerMedCoE optimises key software for cell-level simulations to the new preexascale platforms

The PerMedCoE four core applications are:

- **COBRA** for the simulation of cellular metabolism at genome-scale

- **CellNOpt** for modelling signal transduction networks

- **MaBoSS** for stochastic simulations of Boolean models

- **PhysiCell** an agent-based modelling framework for simulating cell-cell interactions
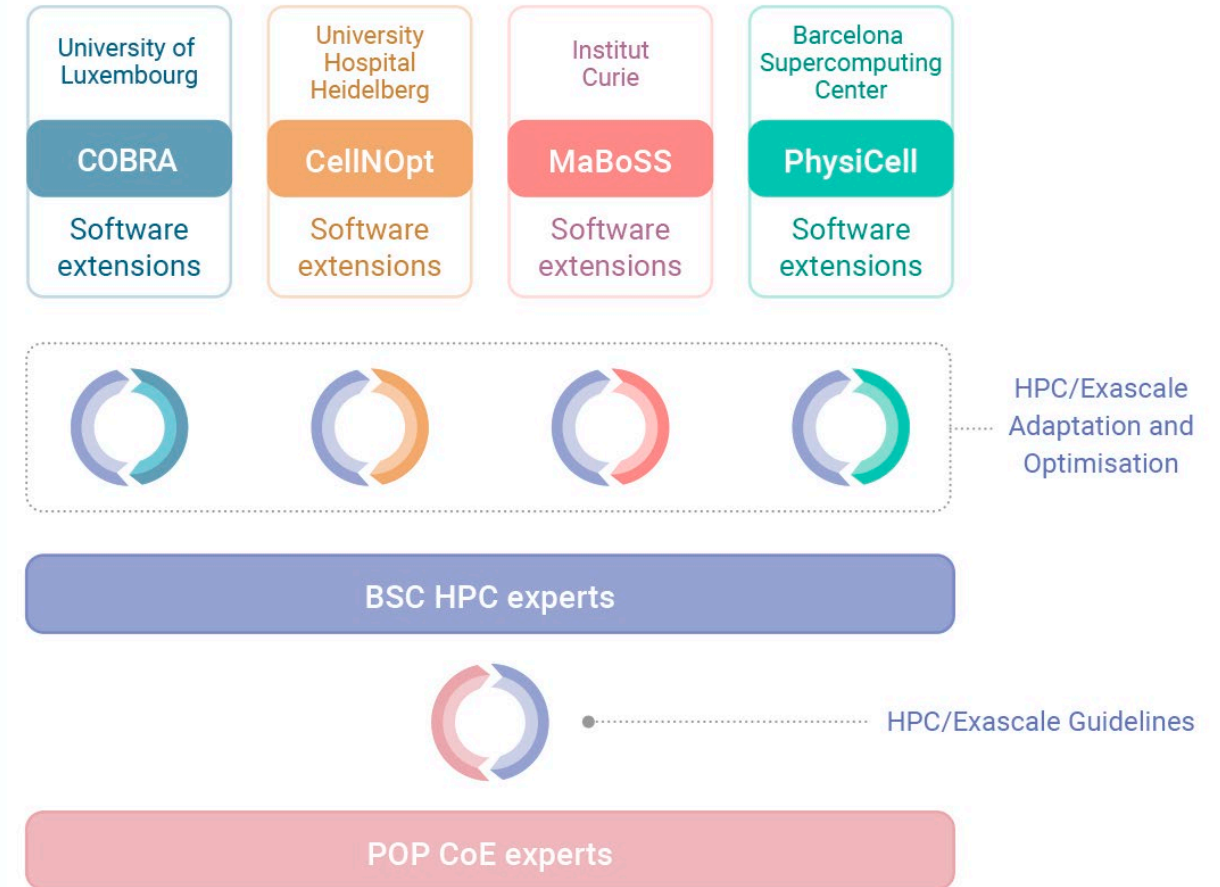
For more information, visit https://permedcoe.eu/core-applications/

USE CASES

PerMedCoE works on five use cases to drive the development of cell-level simulations
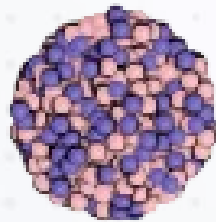
Tumour Evolution
Based on Single-Cell
Omic and Imaging

USE CASES

PerMedCoE works on five use cases to drive the development of cell-level simulations

COVID-19 Multiscale Modelling of the Virus and Patients' Tissue

Cancer Diagnosis Based on Omics Information

Drug Synergies for Cancer Treatment

Tumour Evolution Based on Single-Cell Omic and Imaging

Personalised Modelling of Groups of Rare-Disease Related Patients
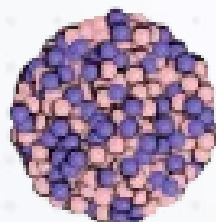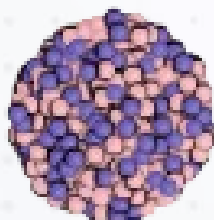
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USE CASES

PerMedCoE works on five use cases to drive the development of cell-level simulations

COVID-19 Multiscale Modelling of the Virus and Patients' Tissue

Cancer Diagnosis Based on Omics Information

Standard Cancer Practice / Hospitals / Health Software Providers

Tumour Evolution Based on Single-Cell Omic and Imaging

Cancer Research / Biotech & Omic to Organois based

Drug Synergies for Cancer Treatment

Clinical Trials / Pharma

Personalised Modelling of Groups of Rare-Disease Related Patients

Rare Diseases / EU Health Systems & Patient Organisation

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