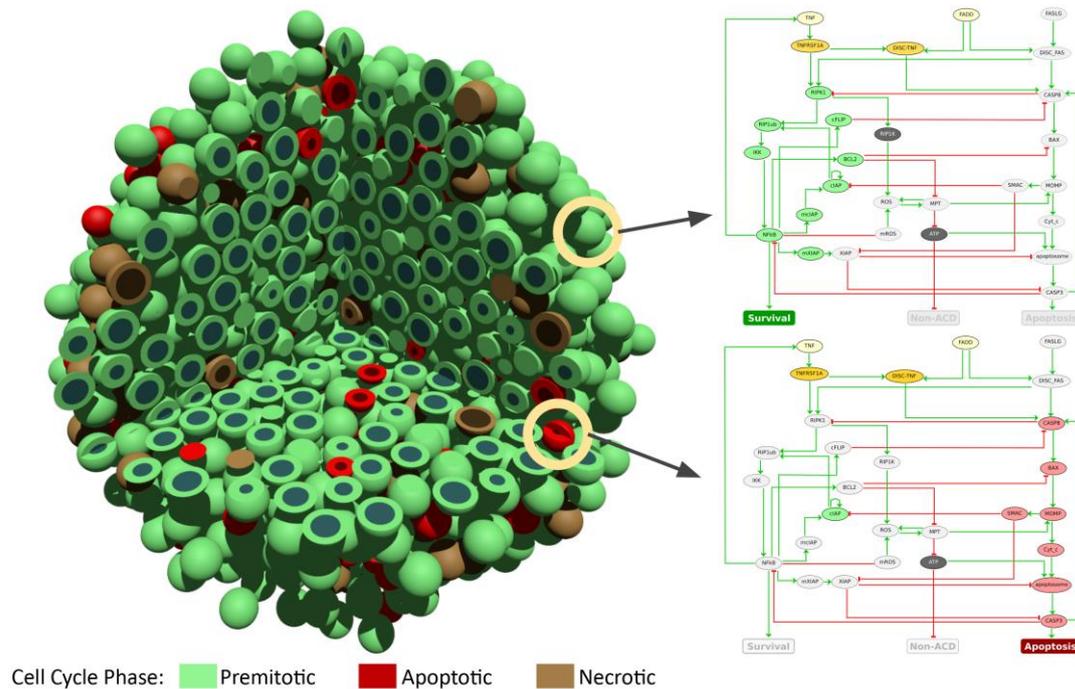


PerMedCoE: Exascale-ready cell-level simulations for European Personalised Medicine

Coordinated by the Barcelona Supercomputing Center (BSC) and funded by the European Commission, this recently launched HPC/Exascale centre of excellence will optimise codes for cell-level simulations in HPC/Exascale and bridge the gap between organ and molecular simulations, thus contributing to the European Personalised Medicine Roadmap.



Example of the framework that enables multiscale simulations. PerMedCoE will allow the scaling-up of multiscale simulations that combine Boolean models that capture intracellular behaviours and agent-based models that study population dynamics. Image by Miguel Ponce de León (PerMedCoE)

The next generation of Exascale supercomputers will become a necessary tool to treat diseases on an individual level and make one step forward in personalised medicine. The recently launched European HPC/Exascale Centre of Excellence in Personalised Medicine (PerMedCoE) will provide an efficient and sustainable infrastructure to support the development of personalised medicine by showcasing HPC/Exascale-upgraded use cases such as translating the consequences of single cell omics information into actionable molecular disease models.

One of the most significant contributions of PerMedCoE will be to scale-up cell-level simulations to HPC/Exascale level, which will fill the gap between the molecular- and organ-level simulations provided by other Centres of Excellence (CoEs) such as [CompBioMed](#) and [BioExcel](#).

“PerMedCoE will boost the competitiveness of European personalised medicine and aims to become the community hub for Exascale-ready software in this domain”, says [Alfonso Valencia](#), ICREA Research Professor, BSC Life Sciences Department Director and PerMedCoE Coordinator.

Personalised medicine opens unexplored frontiers to treating diseases at the individual level combining clinical and omics information. However, the performance of the current simulation



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software is still insufficient to tackle medical problems such as tumour evolution and response to treatment at the single-cell level or patient-specific treatments. For this reason, this European centre of excellence pursues the following main objectives:

- To optimise key software for cell-level simulations to the new pre-exascale platforms to contribute to the European Personalised Medicine Roadmap.
- To integrate personalised medicine into the new European HPC/Exascale ecosystem, by offering access to HPC/Exascale-adapted and optimised software.
- To design and complete a comprehensive set of personalised medicine use cases to drive the development of cell-level simulations.
- To build the basis for its sustainability by coordinating personalised medicine and HPC communities, and reaching out to industrial and academic end-users with use cases, training, expertise and best practices.

The centre will become the entry point to Exascale-ready cell-level simulation software, able to transform personal omics data into actionable mechanistic models of medical relevance, supporting developers and end-users with know-how and best practices. It will also connect simulation software developers with HPC, HTC and HPDA experts at the CoEs [POP](#) and [HiDALGO](#), and work with other biomedical consortia such as [ELIXIR](#) and [LifeTime](#), also connecting pre-exascale infrastructures hosted by supercomputing centres such as the [BSC](#) and [CSC – IT Center for Science](#).

About PerMedCoE

PerMedCoE is the HPC/Exascale Centre of Excellence for Personalised Medicine in Europe and aims to provide an efficient and sustainable entry point to the HPC/Exascale-upgraded methodology to translate omics information into actionable models of cellular functions of medical relevance. Coordinated by the Barcelona Supercomputing Center (BSC), this CoE has been awarded €5 million in funding from the European Commission and will run from 1 October 2020 to 30 September 2023. A range of 12 world-class academic and industry partners from across Europe are participating in the CoE: [Barcelona Supercomputing Center](#) (BSC), [CSC – IT Center for Science](#), [University of Luxembourg](#), [Institut Curie](#), [University Hospital Heidelberg](#), [Atos Spain](#), [KTH Royal Institute of Technology](#), [European Molecular Biology Laboratory](#) (EMBL), [Centre for Genomic Regulation](#) (CRG), [Max Delbrück Center for Molecular Medicine](#) (MDC), [University of Ljubljana](#) and [ELEM Biotech](#).

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