

[PerMedCoE: HPC/Exascale Centre of Excellence on Personalised Medicine](#)

Description

Personalised Medicine (PerMed) opens unexplored frontiers to treat diseases at the individual level combining clinical and omics information. However, the performances of the current simulation software are still insufficient to tackle medical problems such as tumour evolution or patient-specific treatments. 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. 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. The goal of the HPC/Exascale Centre of Excellence in Personalised Medicine (PerMedCoE) is to provide an efficient and sustainable entry point to the HPC/Exascale-upgraded methodology to translate omics analyses into actionable models of cellular functions of medical relevance. It will accomplish so by

- 1) optimising four core applications for cell-level simulations to the new pre-exascale platforms;
- 2) integrating PerMed into the new European HPC/Exascale ecosystem, by offering access to HPC/Exascale-adapted and optimised software;
- 3) running a comprehensive set of PerMed use cases; &
- 4) building the basis for the sustainability of the PerMedCoE by coordinating PerMed and HPC communities, and reaching out to industrial and academic end-users, with use cases, training, expertise, and best practices.

The PerMedCoE cell-level simulations will fill the gap between the molecular- and organ-level simulations from the CompBioMed and BioExcel CoEs with which this proposal is aligned at different levels. It will connect methods developers with HPC, HTC and HPDA experts (at POP and HiDALGO CoEs). Finally, the PerMedCoE will work with biomedical consortia (i.e. ELIXIR, LifeTime initiative) and pre-exascale infrastructures (BSC and CSC), including a substantial co-design effort.

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