Virtual BSC RS/ PerMedCoe Webinar: Exascale-ready cell-level simulations for European Personalised Medicine

Objectives

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

Abstract:
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 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:

- Optimising four core applications for cell-level simulations to the new pre-exascale platforms;
- Integrating PerMed into the new European HPC/Exascale ecosystem, by offering access to HPC/Exascale-adapted and optimised software;
- Running a comprehensive set of PerMed use cases including simulations of tumour evolution and drug combinations for cancer treatment; &
- 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 other CoEs with which this project is aligned at different levels. It will connect method developers with HPC, HTC and HPDA experts. Finally, PerMedCoE will work with biomedical consortia and pre-exascale infrastructures, including a substantial co-design effort.

We hope you will find this topic interesting and will join us for this first session. We would like to remind you that this webinar is the first of of a set of **PerMedCoE webinars** that are open to everyone interested in our tools and activities. The webinars will include a 30-40 minutes presentation and a Q&A section of around 15 minutes. You will find all webinars here: **https://permedcoe.eu/category/training/** and you are able to register for free. All PerMedCoE webinars will be made available on the **project's YouTube channel**, on a dedicated playlist.

More details will come soon!

Speakers

Alfonso Valencia, Barcelona Supercomputing Center, Life Sciences department director
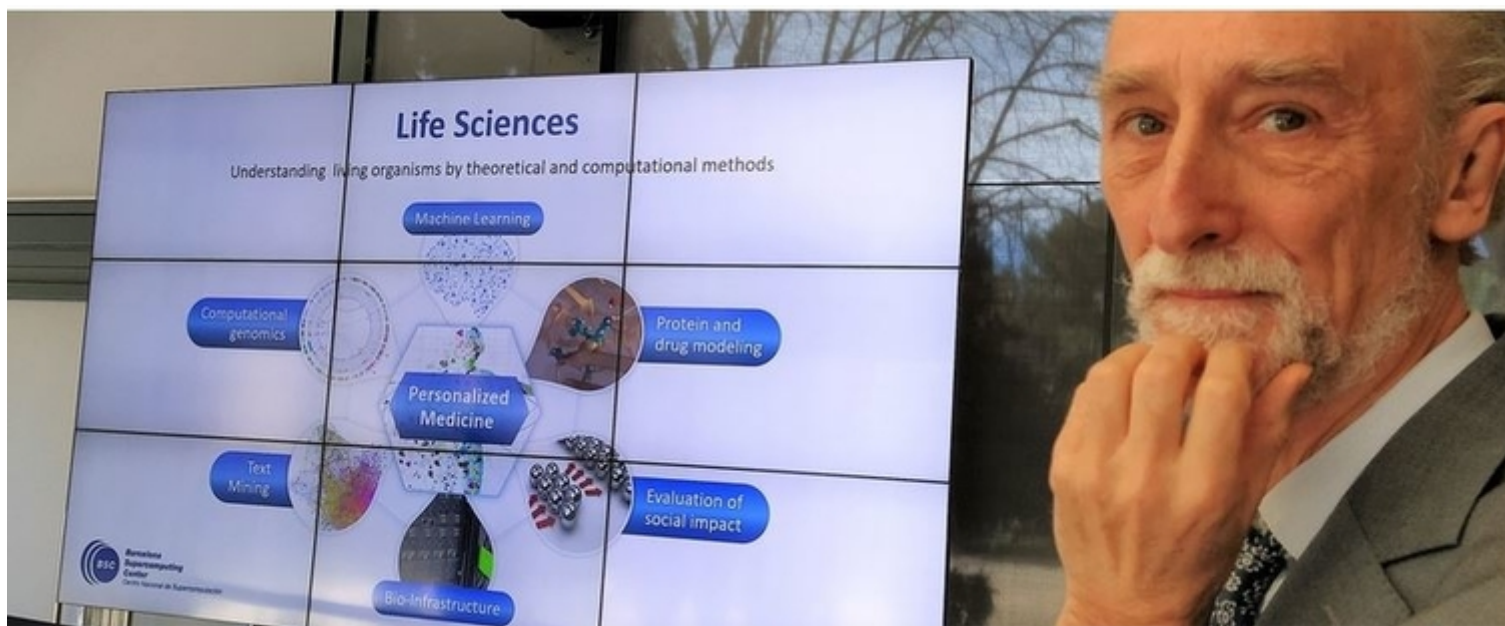
Short Bio: Spanish biologist, ICREA Professor, current director of the Life Sciences department at Barcelona Supercomputing Center (BSC) and of Spanish National Bioinformatics Institute (INB-ISCIII). Alfonso Valencia received his PhD in molecular biology in 1988 from the Autonomous University of Madrid. From 1989 to 1994 he was a Postdoctoral Fellow in the laboratory of Chris Sander at the European Molecular Biology Laboratory (EMBL) in Heidelberg, studying the evolution of protein function using sequence- and structure-based approaches. In 1994 Valencia formed the Protein Design Group at the Spanish National Center for Biotechnology (CNB). He was leader of the Structural and Computational Biology Group at Spanish National Cancer Research Center (CNIO). From 2015-2018, he was President of the International Society for Computational Biology (ISCB). As computational biologist, the focus of his work is the mechanistic understanding of biological systems, including cancer and other diseases, with a combination of Bioinformatics, Network Biology and Machine Learning approaches. His group has developed systems in the areas of protein structure prediction, protein interactions and protein networks, systems biology, text and data mining, with applications in epigenetic, cancer genomics and disease comorbidity. All these activities converge into the general topic of Personalised Medicine, with particular interest in the interface with Artificial intelligence and High Performance Computing.
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