

# 10<sup>th</sup> International BSC Severo Ochoa Doctoral Symposium

9<sup>th</sup> - 10<sup>th</sup> May 2023





## **PROGRAM**

### DAY 1 (May 9th)

Start

time	Activity	Speaker/s	Chair		
8.30h Registration					
9.00h	Welcome and opening	Josep Mª Martorell, BSC Associate Director	Maria Ribera Sancho		
9.20h	Keynote talk: The quest for the quantum computer	Alba Cervera-Lierta, Senior Researcher at the Barcelona Supercomputing Center and Quantum Spain project coordinator			
	Abstract:In this talk, I will explain the brief history of quantum technologies, with particular emphasis on neterm quantum computation, where we are, and the challenges and applications of this technological revolution.				

#### 10.30h Event Photo

#### 10.40h Coffee break & First Poster Session

Spatially-resolved multiscale models shed light into personalized drug treatments, **Alejandro Madrid Valiente** (LS)

Characterizing the Impact of Graph-Processing Workloads on Modern CPU's Cache Hierarchy, **Alexandre Valentin Jamet** (CS)

Representational Learning for the Study of Breast Cancer Progression through Pseudo-Time, **Guillermo Prol Castelo** (LS)

#### 11.40h First Talk Session: Genomics

11.40h 12.00h	Horizontal Gene Transfer in Asgard Archaea, <b>Saioa Manzano-Morales</b> (LS)  Exhaustive Variant Interaction Analysis using Multifactor Dimensionality Reduction, <b>Gonzalo</b>	
12.20h	Gómez (CS) Antibody-Derived Tag normalization for ASAP andscCUT&TAG-PRO, Xavier Soler-Sanchis (LS)	Toni Gabaldón
12.40h	Microbiome profiling from Fecal Immunochemical Test reveals microbial signatures with potential for Colorectal Cancer screening, <b>Olfat Khannous-Lleiffe</b> (LS)	

#### 13.00h Lunch Break

#### 14.00h Tutorial

"Cross-Departmental Collaboration at BSC: Success Stories and a Workshop"

Alba Jené (Bioinformatics Unit Coordinator, LS), Carlos García and Guillermo Marin (Data Pre&Post Processing Researchers, CASE) and Daniele Lezzi (Workflows and Distributed Computing Established Researcher, CS)

The objective of this tutorial is to learn about the potential of cross-departamental collaborations and discover who you could collaborate with.

14:00h - 15:00h Speakers will present several cross-departmental collaborations at BSC and share tips and advice on how to network and collaborate.

15:30h - 17:30h Hands-on workshop: Discover who you could collaborate with.

Following a speed-dating structure, participants will have 6' to share one-on-one informal discussions with peer colleagues to ask questions and explore specific areas of their research and practices (several rounds of discussions). The aim is to find a person to collaborate with or to explore what others do to engage in a potential future collaboration.

#### 17.30h Adjourn

#### **DAY 2 (May 10th)**

Start time	Activity	Speaker/s	Chair
9.00h	Opening of the second day		
9.10h	Second Talk Session: Simulations and Mode	lling	
9.10h	Consensus Essential Dynamics Analysis: Applic (LS)	ation to Biomolecular Simulations, <b>Luis Jord</b> à	à
9.30h	Understanding North Atlantic deep-water format <b>Eneko Martin-Martinez</b> (ES)	ondrivers in an eddy-resolving climate model,	
9.50h	Towards data driven reduced order models for the Franch (CASE)	ne automotive industry, <b>Benet Eiximeno</b>	Sara Royuela
10.10h	Climate Services Ecosystems: What Are They a Gonzalez Romero (ES)	nd Why Are They Are Important?, Carmen	
10.30h	Fault-tolerant applications through OpenMP, Ad	rián Munera (CS)	
40 501	O		

#### 10.50h Coffee break & Second Poster Session

Open-Source GEMM Hardware Kernels Generator: Toward Numerically-Tailored Computations, **Louis Ledoux** (CS)

Prediction of Bacterial Interactomes Based on Genome-Wide Coevolutionary Networks: an Updated Implementation of the ContextMirror Approach, **Miguel Fernández** (LS)

Parallelizing Recurrent Neural Networks and variantsusing OmpSs, Robin Sharma (CS)

Scaling RTL Simulations with Metro-MPI, Guillem López Paradís (CS)

Sorting Impact in Decision Support Benchmarks TPC-H and TPC-DS for Row-Oriented Relational Databases, Iván Vargas Valdivieso (CS)

11.40h	Third Talk Session: Medical and Health Applications		
11.40h	Recapitulating experimental drug synergies in AGSthrough multiscale agent-based simulations, <b>Othmane Hayoun-Mya</b> (LS)		
12h	What is the Added Value of Climate Information for Predicting Infectious Disease Outbreaks,  Chloe Fletcher (ES)  Valentina del Olmo		
12.20	Machine Learning approaches for thecharacterization of COPD, Iria Pose Lagoa (LS)		
12.40	Ranking Allosteric Activators of AMPK by Absolute Binding Free Energy Calculations with FunmetaD, <b>Rhys Evans</b> (LS)		
13.00h	Lunch Break		
14:00h	Fourth Talk Session: Tools Development		
14:00h	NTRU Cryptosystem: A solution to the quantum threat, <b>Miquel Guiot Cusidó</b> (CS)		
	JLOH: Inferring Loss of Heterozygosity Blocks fromShort-Read Sequencing Data, Matteo		
14:20h	Schiavinato (LS)		
4.4.401	VAQUERO: A Scratchpad-based Vector Acceleratorfor Query Processing, <b>Julián Pavón</b> Petar		
14:40h	Rivera (CS)  TIGER: The gene expression regulatory variation landscape of human pancreatic islets,		
15:00h	Lorena Alonso (LS)		
10.0011	A Stochastic Method for Solving Time-Fractional Differential Equations, <b>Nicolas L. Guidotti</b>		
15:20h	(CS)		
15.40h	Coffee break & Third Poster Session		
	Variability of univariate and compound hot and dry events, <b>Alvise Aranyossy</b> (ES)		
	A Stroke Risk Assessment Tool for Edge-to-Cloud Platforms, Fatemeh Baghdadi (LS)		
	Multi-model Forecast Quality Assessment of CMIP6 Decadal Predictions, <b>Carlos Delgdo-Torres</b> (ES - Earth System Services)		
	Numerical analysis of MHD flow of magnetically confined plasma in cylindrical geometry usingOpenFOAM, <b>Robert Benassai</b> (CASE)		
	In Silico Bioprospecting of Enzymatic PEF Synthesis and Degradation, Rubén Muñoz Tafalla (LS)		
16.40h	Fifth Talk Session: Artificial intelligence and its Aplications		
16:40h	Multi-dimensional Fourier series with quantum circuits, Berta Casas Font (CASE)		
17:00h	Tailored Molecular Modelling and Machine Learning solutions for small-molecule drug discovery, Isaac Filella Merce (LS)  Artur García		
17:20h	New Tensor Network Structures in 1.5D, Sergi Masot Llima (CASE)		
17:40h	DNN Acceleration in the limits of Energy Efficiency, <b>Jordi Fornt</b> (CS)		
18.00h	Final remarks and End of Doctoral Symposium		
18:20h	Cool off		