



PROGRAM

DAY 1 (May 9th)

| Start time | Activity | Speaker/s | Chair |
|------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------|----------------------------|
| 8.30h | Registration | | |
| 9.00h | Welcome and opening | Josep M^a Martorell , BSC Associate Director | Maria Ribera Sancho |
| 9.20h | Keynote talk: The quest for the quantum computer Abstract: In this talk, I will explain the brief history of quantum technologies, with particular emphasis on near-term quantum computation, where we are, and the challenges and applications of this technological revolution. | Alba Cervera-Lierta , Senior Researcher at the Barcelona Supercomputing Center and Quantum Spain project coordinator | |
| 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) | | |
| | Multi-annual predictions of daily temperature and precipitation extremes, Carlos Delgado-Torres (ES) | | |
| | 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 | Horizontal Gene Transfer in Asgard Archaea, Saioa Manzano-Morales (LS) | | |
| 12.00h | Exhaustive Variant Interaction Analysis using Multifactor Dimensionality Reduction, Gonzalo Gómez (CS) | | |
| 12.20h | Antibody-Derived Tag normalization for ASAP and scCUT&TAG-PRO, Xavier Soler-Sanchis (LS) | | Toni Galabón |
| 12.40h | Microbiome profiling from Fecal Immunochemical Test reveals microbial signatures with potential for Colorectal Cancer screening, Olfat Khannous-Lleiffe (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-departmental 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 Modelling | | |
| 9.10h | Consensus Essential Dynamics Analysis: Application to Biomolecular Simulations, | Luis Jordà (LS) | |
| 9.30h | Understanding North Atlantic deep-water formation drivers in an eddy-resolving climate model, | Eneko Martin-Martinez (ES) | |
| 9.50h | Towards data driven reduced order models for the automotive industry, | Benet Eiximeno Franch (CASE) | Sara Royuela |
| 10.10h | Climate Services Ecosystems: What Are They and Why Are They Are Important?, | Carmen Gonzalez Romero (ES) | |
| 10.30h | Fault-tolerant applications through OpenMP, | Adrián Munera (CS) | |
| 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 variants using OmpSs, | Robin Sharma (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 AGS through multiscale agent-based simulations, **Othmane Hayoun-Mya** (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 the characterization of COPD, **Iria Pose Lagoa** (LS)

12.40 Ranking Allosteric Activators of AMPK by Absolute Binding Free Energy Calculations with Fun-metaD, **Rhys Evans** (LS)

13.00h Lunch Break**14:00h Fourth Talk Session: Tools Development**

14:00h NTRU Cryptosystem: A solution to the quantum threat, **Miquel Guiot Cusidó** (CS)

14:20h JLOH: Inferring Loss of Heterozygosity Blocks from Short-Read Sequencing Data, **Matteo Schiavinato** (LS)

14:40h VAQUERO: A Scratchpad-based Vector Accelerator for Query Processing, **Julián Pavón Rivera** (CS)

Petar Radojkovic

15:00h TIGER: The gene expression regulatory variation landscape of human pancreatic islets, **Lorena Alonso** (LS)

15:20h A Stochastic Method for Solving Time-Fractional Differential Equations, **Nicolas L. Guidotti** (CS)

15.40h Coffee break & Third Poster Session

Variability of univariate and compound hot and dry events, **Alvise Aranyossy** (ES)

A Stroke Risk Assessment Tool for Edge-to-Cloud Platforms, **Fatemeh Baghdadi** (LS)

Multi-model Forecast Quality Assessment of CMIP6 Decadal Predictions, **Carlos Delgado-Torres** (ES - Earth System Services)

Numerical analysis of MHD flow of magnetically confined plasma in cylindrical geometry using OpenFOAM, **Robert Benassai** (CASE)

In Silico Bioprospecting of Enzymatic PEF Synthesis and Degradation, **Rubén Muñoz Tafalla** (LS)

16.40h Fifth Talk Session: Artificial intelligence and its Applications

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, **Jordi Fornt** (CS)

18.00h Final remarks and End of Doctoral Symposium**18:20h Cool off**