



PROGRAM

DAY 1 (24th of April)

Start time	Activity	Speaker/s	Chair
8.30h Registration			
9.00h	Welcome and opening	Josep M ^a Martorell, BSC Associate Director	
9.20h	Keynote talk: Quantum Disruption	Jose Ignacio Latorre Sentis Quantic Group Leader, CASE, BSC	Maria-Ribera Sancho
<p>Abstract: Quantum Technologies are coming of age. The EU has recently approved a FET-Flagship on Quantum Technologies, an instrument that will invest 1000 M Euros structured around four pillars: quantum computation, quantum communication, quantum simulation and quantum sensors. In this talk, we shall concentrate in recent progress achieved in quantum computation. The basic idea emerges from the fact that quantum mechanics allows for the manipulation of information in superposition states, called qubits. Furthermore, these superpositions evolved simultaneously following logical gates, providing a genuine parallel computation paradigm. A relevant example of the future use of a quantum computer is illustrated by Shor's algorithm, a quantum circuit that will factor large numbers in polynomial time, and will consequently break all present cryptography. Quantum logic, though, does not correlate in a simple way to classical algorithms. Non-trivial efforts must be devoted to further understand which problems can be addressed efficiently with quantum computation. Finally, it is arguable that quantum computation brings not only a possible dramatic speed up in some computations, but also provides relevant savings in energy. Research teams around the world compete fiercely to get a first demonstration of quantum supremacy over classical computation. Welcome to the quantum race.</p>			
10.30h Event Photo			
Coffee break & First Poster Session			
10.40h	<ol style="list-style-type: none"> Application of the edge-based finite element method for fusion plasma simulations, Marc Fuster Skip RNN Learning to Skip State Updates in Recurrent Neural Networks, Víctor Campos Recurrent Semantic Instance Segmentation, Miriam Bellver Improving Time-Randomized Cache Designs, Pedro Benedicte Co-Evolution of Morphology and Behavior in Self-Organized Robotic Swarms, Jessica Meyer 		
First Talk Session: Life Sciences			
11.40h	FrAG-PELE: Novel Fragment-based Growing Tool for hit-to-lead in Early Drug Discovery	Carles Pérez López	David Torrents

12.00h Sampling Interfacial Water Effects over Protein Specificity with PELE Marti Municoy Terol

12:20h Characterization of pathological mutations affecting protein-protein interactions for drug discovery Mireia Rosell Oliveras

12.40h Lunch Break

14.30h Tutorial 1

Title: Troubleshooting Session: Key challenges for early-career researchers Gavin Lucas PhD, director of ThePaperMill

Goals & Content

The goal of this short session is help early-career researchers gain new perspectives on some of the key challenges they face, and to acquire practical tools that they can apply in their day-to-day working environment. I will present short modules focused on communication, personal effectiveness, and on sharing and discussing the common challenges faced by all early career researchers, and how they can be addressed.

Topics for this workshop:

- Group awareness - Troubleshooting the challenges of early-career research
- Communication - Understanding my audience and pitching my message
- Project Management – How can I prioritise my tasks?

16.30h Adjourn

DAY 2 (25th of April)

Start time	Activity	Speaker/s	Chair
9.00h	Opening of the second day		
Second Talk Session: Simulations and Modelling			
9.10h	Comparison of seismic ground motions in Mexico City due to damaging earthquakes applying Seismograms Analyzer-e	Armando Aguilar-Melendez	Josep Casanovas
9.30h	Earthquake simulation by Fiber Bundle Model and Machine Learning techniques	Marisol Monterrubio Velasco	
9.50h	An introduction to FE2 multi-scale methods and why HPC is so crucial.	Guido Giuntoli	
10.10h	Effect of population structure, parameter estimation of complex model, and effect of LITB on TB dynamics	Nura Mohammad Rabiuh Ahmad	
10.30h	An assessment of regional sea ice predictability in the Arctic ocean	Ruben Cruz-García	

10.50h Coffee break & Second Poster Session:

1. A Unified Memory approach to GPU acceleration on task based programming models, Aimar Rodríguez
2. A Machine Learning Workflow for Hurricane Prediction, Albert Kahira
3. Evaluation of traffic emission models coupled with a microscopic traffic simulator and on-road measures, Daniel Rev
4. Accelerating binding free energy calculations by combining Monte Carlo simulations, enhanced sampling and Markov State Models, Joan Francesc Gilabert

Third Talk Session: Programming Models and Computer Architectures

12.00h	Model-based Machine Learning for Retrospective Event Detection	Joan Capdevila Pujol	Eduard Ayguadé
12.20h	Detailed Tuning and Validation of Hardware Simulators through Microbenchmarks	Rommel Sánchez	
12.40h	Enabling a Reliable STT-MRAM Main Memory Simulation	Kazi Asifuzzaman	
13.00h	A Linux Kernel Scheduler Extension for Multi-Core Systems	Aleix Roca Nonell	

13 20h Lunch break**14.30h Tutorial 2**

Title: How to become rich following an academic career	Leonardo Bautista-Gomez, Research Scientist at BSC
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Content&Goals

The scientific field is very competitive and sometimes it can be even intimidating. This can lead promising young researchers to move to other domains or industries. However, following an academic career also comes with multiple advantages that might be hard to recognize at the early stages. In this talk I will present the perks and benefits of following an academic career.

Title: Marie Curie Individual Fellowships: Info & Best Practices	Toni Peña, Sr. Researcher at BSC
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Content&Goals

Marie Skłodowska-Curie Individual Fellowships from the European Commission are a great hit in a researcher's career. We will introduce these fellowships, including requirements and benefits, and will advise on how to prepare a successful application.

15.40h Coffe break

Fourth Talk Session: Algorithms and applications

16.00h	Modelling of Alfvénic instabilities in complex toroidal magnetic geometries for fusion	Allah Rakha	Osman Unsal
16.20h	Robust point-location method for linear and high order meshes. Application to particle transport	Edgar Olivares	
16.40h	On the quest to reach nuclear fusion as a future energy source	Dani Gallart Escolà	
17.00h	Fuzzy Finite State Machines in Crowd Simulation	Leonel Antonio Toledo Díaz	
17.20h	Top View Human Head and Shoulder Classification Using CNN	Ivan Rivalcoba	
17.40h	Conclusions		

17.50 End of the Doctoral Symposium