



PROGRAM

DAY 1 (May 7th)

| Start time | Activity | Speaker/s | Chair |
|--|--|--|---------------------|
| 8.30h Registration | | | |
| 9.00h | Welcome and opening | Sergi Girona , BSC Operations Director and CIO | Maria Ribera Sancho |
| 9.20h | Keynote talk: Brain and behaviour: to which extent are we responsible for who we are? | David Bueno i Torrens , Universitat de Barcelona (UB) | |
| | <p>Abstract: The brain is the organ of thought. Its neural networks manage all our behaviours. Its ontogenetic origin, however, is dual. On one hand, its formation and its functioning are conditioned by a number of genes, which make each person more or less prone to any cognitive ability as well as for any behavioural response. On the other hand, the environment also influences how the synaptic connections are established, which in turn sets the neural networks, whose activity will generate all the behaviours and learning. What is the relative influence of each of these factors? Can we contribute to the construction of our brain? In this keynote we will discuss to which extent we are responsible for being who we are.</p> | | |
| 10.30h Event Photo | | | |
| Coffee break & First Poster Session | | | |
| | Development of HPC Multiphysics Framework for HTS Magnets in Fusion, José Lorenzo | | |
| | Deciphering the interactions between the immune system and cancer cells to enable precision medicine, Victoria Ruiz-Serra | | |
| | Local traffic contribution to black carbon horizontal and vertical profiles in compact urban areas, Jaime Benavides | | |
| | De novo binding prediction of peptides to MHC class I, Pep Amengual-Rigo | | |
| 10.40h | PluriZymes: new enzymes for new times, Marc Domingo Cabasés | | |
| 11.40h | First Talk Session: Algorithms, plastic biodegradation, wave propagation and seismology | | |
| | 1. Towards PET degradation engineering | Sergi Rodà | |
| | 2. Maximal Entanglement in Quantum Computation | Alba Cervera | |
| | 3. Solving Parameteric Wave Propagation Models with Domain Decomposed Reduced Order Methods | Prattya Datta | Victor Guallar |

4. Multifractal characterization of seismicity: the case of Carterbury region (New Zealand), 2000-2018 **Marisol Monterrubio Velasco**

13.00h Lunch Break

14.00h Tutorial 1st part

Creativity & Innovation: Why creativity is needed in a science career? **Alicia Marín Muniesa, Isabel Nogueroles, Judit Murlans**

Goals & Content

Goal: The goal of this workshop is to set the scene to value creativity and innovation in a scientific environment.

Contents:

Creative Thinking:

Creativity vs. Innovation

Uses in the scientific environment

Requirements and strategies to foster creativity and innovation

Barriers and blockages

Practices and resources to develop creativity and innovation

Collecting challenges to solve them with the help of creativity techniques

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?

16.00h Adjourn

DAY 2 (May 8th)

| Start time | Activity | Chair |
|------------|---|--|
| 9.00h | Opening of the second day | |
| 9.10h | Keynote talk 2: Preparing for Extreme Heterogeneity in High Performance Computing | Jeffrey Vetter , Oak Ridge National Laboratory (ORNL) Petar Radojkovic |
| | <p>Abstract: While computing technologies have remained relatively stable for nearly two decades, new architectural features, such as heterogeneous cores, deep memory hierarchies, non-volatile memory (NVM), and near-memory processing, have emerged as possible solutions to address the concerns of energy-efficiency and cost. However, we expect this ‘golden age’ of architectural change to lead to extreme heterogeneity and it will have a major impact on software systems and applications. Software will need to be redesigned to exploit these new capabilities and provide some level of performance portability across these diverse architectures. In this talk, I will sample these emerging memory technologies, discuss their architectural and software implications, and describe several new approaches (e.g., domain specific languages, intelligent compilers and introspective runtime systems) to address these challenges.</p> | |

10.20h Coffee break & Second Poster Session:

An ILP-based Real-Time Scheduler for Distributed and Heterogeneous Computing Environments, **Eudald Sabaté Creixell**

Techniques for reducing and bounding OpenMP dynamic memory, **Adrián Munera Sánchez**

C/R Support for Heterogeneous HPC Applications, **Konstantinos Parasyris**

High-Integrity GPU Designs for Critical Real-Time Automotive Systems, **Sergi Alcaide Portet**

11.30h Second Talk Session: Data Analytics, genetic variability, distributed computing and seismology

1. Orchestration of Software Packages in Data Science Workflows

Cristian Ramon-Cortes Vilarrodona

2. Characterization of Structural Genomic Variability in Population Cohorts

Jordi Valls

Rosa Badia

3. Cyberinfrastructure programming with COMPs

Francesc Lordan

4. Assessment of Damage Potential of Seismic Ground Motions

Armando Aguilar Meléndez

13.00h Lunch Break

14.00h Third Talk Session: Machine Learning, personalized medicine and air quality

1. Analysis of the interaction of genomic variants and their association to common diseases

Lorena Alonso Parrilla

2. Correcting Air Quality Forecasts with Machine Learning Algorithms

Hervé Petetin

Eduard Ayguadé

3. TauRieL: Targeting Traveling Salesman Problem with deep reinforcement learning

Gorker Alp Malazgirt

4. Training CNNs using high-resolution images of variable shape

Ferran Parés Pont

15.30h Tutorial session 2

Creativity & Innovation: Working on real challenges with Design Thinking techniques

Alicia Marín Muniesa, Isabel Nogueroles, Judit Murlans

Content&Goals Goal: The goal of this workshop is to provide scientists with practical tools and resources that can be applied in their working environment to bring innovation to life.

Contents:

Presenting challenges to be solved in teams

The process of creative problem solving

Introducing and practicing with applied creativity techniques:

Design Thinking (IDEO)

Design Sprint (GOOGLE)

Participants present their creative solutions

Individual Action Plan to transfer learning to the workplace

17.30h Adjourn

DAY 3 (May 9th)

| Activity | Chair | |
|--|-----------------------------------|-------------------|
| 9.00h Opening of the third day | | |
| 9.10h Fourth Talk Session: HPC, biological simulation and computer architecture | | |
| 1. Containers in HPC: A Scalability and Portability Study in Production Biological Simulations | Oleksandr Rudy | |
| 2. Exploration of architectural parameters for future HPC systems | Constantino Gómez | |
| 3. Supporting task creation inside FPGA devices | Jaume Bosch | Filippo Mantovani |
| 4. Enhancing Scheduling through Monitoring and Prediction Techniques | Antoni Navarro Muñoz | |
| 5. Experimental Study of Aggressive Undervolting in FPGAs | Behzad Salami | |
| 10.50h Coffee break & Third Poster Session | | |
| A FM-index transformation to enable large k-steps, Rubén Langarita | | |
| A multilayer network approach to elucidate severity in Congenital Myasthenic Syndromes, Iker Núñez | | |
| Deep Learning Phase Picking of Large-N experiments, Luis Fernández-Prieto | | |
| Performance optimization of fully anisotropic elastic wave propagation on 2nd Generation Intel Xeon Phi processors, Albert Farres | | |
| 11.50h Fifth Talk Session: Meshes and Fluids, Hemodynamics | | |
| 1. Towards a low dissipation FE scheme for scale resolving turbulent compressible flows | Lucas Gasparino | |
| 2. Local bisection for conformal refinement of unstructured 4D simplicial meshes | Guillem Belda Ferrín | Arnau Folch |
| 3. Defining a stretching and alignment aware quality measure for linear and curved 2D meshes | Guillermo Aparicio Estrems | |
| 4. A One-Dimensional Finite Element Model for Human Circulatory Systems | David Oks | |
| 13.15 Lunch | | |
| 14.30h Sixth Talk Session: Models and simulation, dust and pathogenicity prediction | | |
| 1. Correctly modeling IR spectra of astronomical interesting nanosilicate clusters | Joan Mariñoso Guiu | |
| 2. How much soil dust aerosol is man-made? | Martina Klose | Enza DiTomaso |
| 3. Structural and Dynamics Analysis of Pyruvate Kinase from Erythrocytes: Implications in Pathology | Luis Jordà | |
| 16.00h Adjourn/End of Doctoral Symposium | | |