PROGRAM

DAY 1 (May 7th)

Start time	Activity	Speaker/s	Chair
8.30h Reg	istration		
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)	
	Abstract: The brain is the organ of thought. Its neural	networks manage all our behaviours. Its ontoge	netic origin

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 conexions 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.

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 Progagation 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	Alicia Marín Muniesa, Isabel Nogueroles, Judit
science career?	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)

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Start time	Activity	Chair
9.00h	Opening of the second day	
9.10h	Keynote talk 2: Preparing for Extreme Heterogeneity Jeffrey Vetter , Oak Ridge National Laboratory in High Performance Computing (ORNL)	Petar Radojkovic
	Abstract: While computing technologies have remained relatively stable for nearly two decades new a	rchitectural

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.

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

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	Lorena Alonso Parrilla	
their association to common diseases		
2. Correcting Air Quality Forecasts with Machine	Hervé Petetin	
Learning Algorithms	nerve retetiii	Eduard Ayguadé
3.TauRieL: Targeting Traveling Salesman Problem	Gorker Alp Malazgirt	
with deep reinforcement learning	Gorker Aip Maiazgirt	70
4. Training CNNs using high-resolution images of		
variable shape	Ferran Parés Pont	

15.30h Tutorial session 2

Creativity & Innovation: Working on real challenges Alicia Marín Muniesa, Isabel Nogueroles, Judit with Design Thinking techniques 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

Enhancing Scheduling through Monitoring and Prediction Techniques	Antoni Navarro Muñoz	
2.Exploration of architectural parameters for future HPC systems	Constantino Gómez	
3. Supporting task creation inside FPGA devices	Jaume Bosch Filip	•
4. Containers in HPC: A Scalability and Portability Study in Production Biological Simulations	Oleksandr Rudyy	
5. Experimental Study of Aggressive Undervolting in	Rehzad Salami	

10.50h Coffee break & Third Poster Session

FPGAs

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

Towards a low dissipation FE scheme for scale resolving turbulent compressible flows	Lucas Gasparino	
2. Local bisection for conformal refinement of unstructured 4D simplical meshes	Guillem Belda Ferrín	
3. Defining a stretching and alignment aware quality measure for linear and curved 2D meshes	Guillermo Aparicio Estrems	Arnau Folch
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	Oriol Jorba
3. Structural and Dynamics Analysis of Pyruvate Kinase from Erythrocytes: Implications in Pathology	Luis Jordà	

16.00h Adjourn/End of Doctoral Symposium