



PROGRAM

DAY 1 (May 10th)

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: Competences as the key to success for strong technological developments Abstract: I will present the idea behind the activity of building National Centres of Excellence in Europe and how it is being implemented. First successes will be presented and the embedding of the network of competence centres in the European HPC ecosystem will be shown. It will also become clear how important competences are in the European HPC strategy and how to interact with the (constantly growing) network at national and European level.	Bastian Koller , Managing Director, HLRS	
10.30h Event Photo			
10.40h Coffee break & First Poster Session			
A platform for antibody design, Anna Maria Díaz-Rovira (LS - Electronic and Atomic Protein Modelling)			
Designing a Cloud and HPC Based M&S platform to Investigate the IVD Diseases Mechanism, Maria Paola Ferri (LS - INB)			
Low Input Promoter Capture Hi-C Method Enables to Decipher the Molecular Mechanisms Underlying Genetically Complex Diseases, Paula López-Martí (LS - Computational Biology Life Sciences)			
FAIRsoft - A practical implementation of FAIR principles for research software, Eva Martín del Pico (LS - INB)			
CSDownscale: an R Package for Statistical Downscaling, Jaume Ramon (ES - Earth System Services)			
JLOH: Extracting Loss of Heterozygosity Blocks from Short-Read Sequencing Data, Matteo Schiavinato (LS - Comparative Genomics)			

(continues)

11.40h First Talk Session: Performance

- 11.40h TACL: Interoperating asynchronous device APIs with task-based programming models, **David Álvarez** (CS - Programming Models)
- 12.00h PredIG: a predictor of T-cell immunogenicity, **Roc Farriol-Duran** (LS - Electronic and Atomic Protein Modelling)
- 12.20h Exploring Task Scheduling Sensitivity to L1 Cache configuration on a 32-core RISC-V Processor, **Lucas Morais** (CS - Computer Architecture for Parallel Paradigms)
- 12.40h Investigating Memory Prefetcher Performance over Parallel Applications: From Real to Simulated, **Valéria Soldera Girelli** (CS - Memory technologies)

**Víctor
Guallar
Tasies**

13.00h Lunch Break**14.00h Tutorial 1st part**

“Effective Team Work and External Collaborations”

Moisés Martínez

The purpose of the workshop is to deliver a tailor made training experience with content and strategies focused on the following:

- how to deal with a director and teammates,
- how to work as a part of a team and independently,
- how to work with people from other institutions,
- how to network and use the scientific community to support your own growth,
- how to deal with conflict.

17.00h Adjourn**DAY 2 (May 11th)**

Start time	Activity	Speaker/s	Chair
9.00h	Opening of the second day		
9.10h	Second Talk Session: Simulations and Modelling 1		
9.10h	The development of high-order methods for finite elements to study turbulent reacting flow,	Antonio Blanco Casares (CASE - Propulsion Technologies)	Eduardo Pérez
9.30h	Implementation of cellular transport models within a multiscale simulation software,	Othmane Hayoun Mya (LS - Computational Biology)	
9.50h	Numerical Investigation of Unsteady Processes in Combustion using Flame Transfer Function,	Phivos Andreou Koumides (CASE - Propulsion Technologies Group)	
10.10h	Non-Reacting Large Eddy Simulation of a Low Swirl Burner,	Fredherico Rodrigues (CASE - Propulsion Technologies)	
10.30h	Coffee break & Second Poster Session		
	Distributed Tabulation of Flamelet Lookup Tables, Nicholas Abel (CASE - Propulsion Technologies)		
	Discovering the Ethereum2 P2P Network, Mikel Cortes Goicoechea (CS - Resilience in Distributed Systems)		
	Multi-model Forecast Quality Assessment of CMIP6 Decadal Predictions, Carlos Delgado-Torres (ES - Earth System Services)		

Ground-Level Ozone Simulations Improved by Updating Land Cover Databases, **Franco López** (ES - Atmospheric Composition)
 Rational Enzyme Engineering of Different Active Sites on a Xylanase, **Rubén Muñoz Tafalla** (LS - Electronic and Atomic Protein Modelling)
 Development of corrections for the absolute free binding energy prediction, **Ignasi Puch-Giner** (LS - Electronic and Atomic Protein Modelling)

11.40h Third Talk Session: Performance 2

11.40h Improving resource usage in large FPGA accelerators, **Antonio Filgueras** (CS - Programming Models)

12h CAMP First GPU Solver: A Solution to Accelerate Chemistry in Atmospheric Models, **Christian Guzman Ruiz** (ES - Computational Earth Sciences)

12.20 b8c: an FPGA-Friendly Sparse Matrix Representation Suitable for the SpMV kernel, **José Oliver Segura** (CS - Programming Models)

12.40 HBM, Present and Future of HPC based on FPGAs, **Elias Augusto Perdomo Hourné** (CS - European Exascale Accelerator)

Eduard Ayguadé

13.00h Lunch Break**14.00h Tutorial session 2**

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17.00h Adjourn**DAY 3 (May 12th)**

Start time	Activity	Speaker/s	Chair
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9.00h Opening of the third day

9.10h Fourth Talk Session: Simulations and Modelling 2

9.10h Numerical Simulations for the Atomic Beam Probe, **Mátyás Aradi** (CASE - Fusion)

9.30h Nuclear Fusion Reactor Materials: Modelling Atomic-Scale Irradiation Damage in Metal, **Mary Kathleen Chessey** (CASE - Fusion)

9.50h Comparison of Five Strategies for Seasonal Prediction of Bioclimatic Indicators in the Olive Sector, **Chihchung Chou** (ES - Earth System Services Group)

Dani Guallart

10.10h	Adaptive points to estimate the Lebesgue constant on the simplex, Albert Jiménez Ramos (CASE - Geometry and Meshing for simulations)	
10.30h	Preparing plasma heating in ITER using integrated modelling, Tomás Bensadon (CASE - Fusion)	
10.50h	Coffee break & Third Poster Session	
	Foreign and domestic contributions to surface ozone on Spain, Roger Garatachea (ES - Atmospheric Composition)	
	Respiratory tract microbiome modifications after lung transplantation and its impact in CLAD, Olfat Khannous (LS - Comparative Genomics)	
	Organic Particle Export, Remineralization and Advection in the North Atlantic mesopelagic layer, M. Andrea Orihuela-García (LS - Climate Prediction)	
	Characterisation of Ozone levels and associated NMVOC emissions in Spain: a preliminary assessment, Kevin Oliveira (ES - Atmospheric Composition)	
	Experimental Analysis on the NXP's T2080 Cache Coherence: A Step Towards MPSoCs in Critical Systems, Roger Pujol Torramorell (CS - Operating System / Computer ArchitectureInterface)	
	Space Shuttle: A Test Vehicle for the Reliability of the SkyWater 130nm PDK using OpenLane and the Google/E-fabless Shuttle Run, Ivan Rodriguez-Ferrandez (CS - Operating System / Computer Architecture Interface)	
11.50h	Fifth Talk Session: Life Sciences	
11.50h	Characterisation of inter-individual genomic variability across populations of different genetic ancestries, Rubén Chazarra Gil (LS - Transcriptomics and Functional Genomics Lab)	
12.10h	Transcriptome Analysis of Differential Gene Expression in Disease, José Miguel Ramírez (LS - Transcriptomics and Functional Genomics Lab)	Raquel García
12.30h	RosneT: A Block Tensor Algebra Library for Out-of-Core Quantum Computing Simulation, Sergio Sánchez Ramírez (CASE - Quantic)	
12.50h	Exploring the recent evolution of yeast pathogens using the CandidaMine database, Miquel Àngel Schikora Tamarit (LS - Comparative Genomics)	
13.10	Lunch	
14.00h	Sixth Talk Session: Machine Learning and its applications	
14.00h	Focus! Rating XAI Methods and Finding Biases, Anna Arias Duart (CS - High Performance Artificial Intelligence)	
14.20h	Reaching a modular, generic and containerized development in Biomedical Natural Language Processing systems, Javier Corvi (LS - INB)	Daniele Lezzi
14.40h	QUARQ QUick Approximate and Relaxed Querying, Victor-Alejandro Ortiz (CASE - Smart Cities)	
15.00h	Hyperparameter Optimization using Agents for Large Scale Machine Learning, Pere Vergés Boncompte (CS - Workflows and Distributed Computing)	
15.20h	Final remarks and End of Doctoral Symposium	

