

Strengthening innovation via scientific and high-performance computing

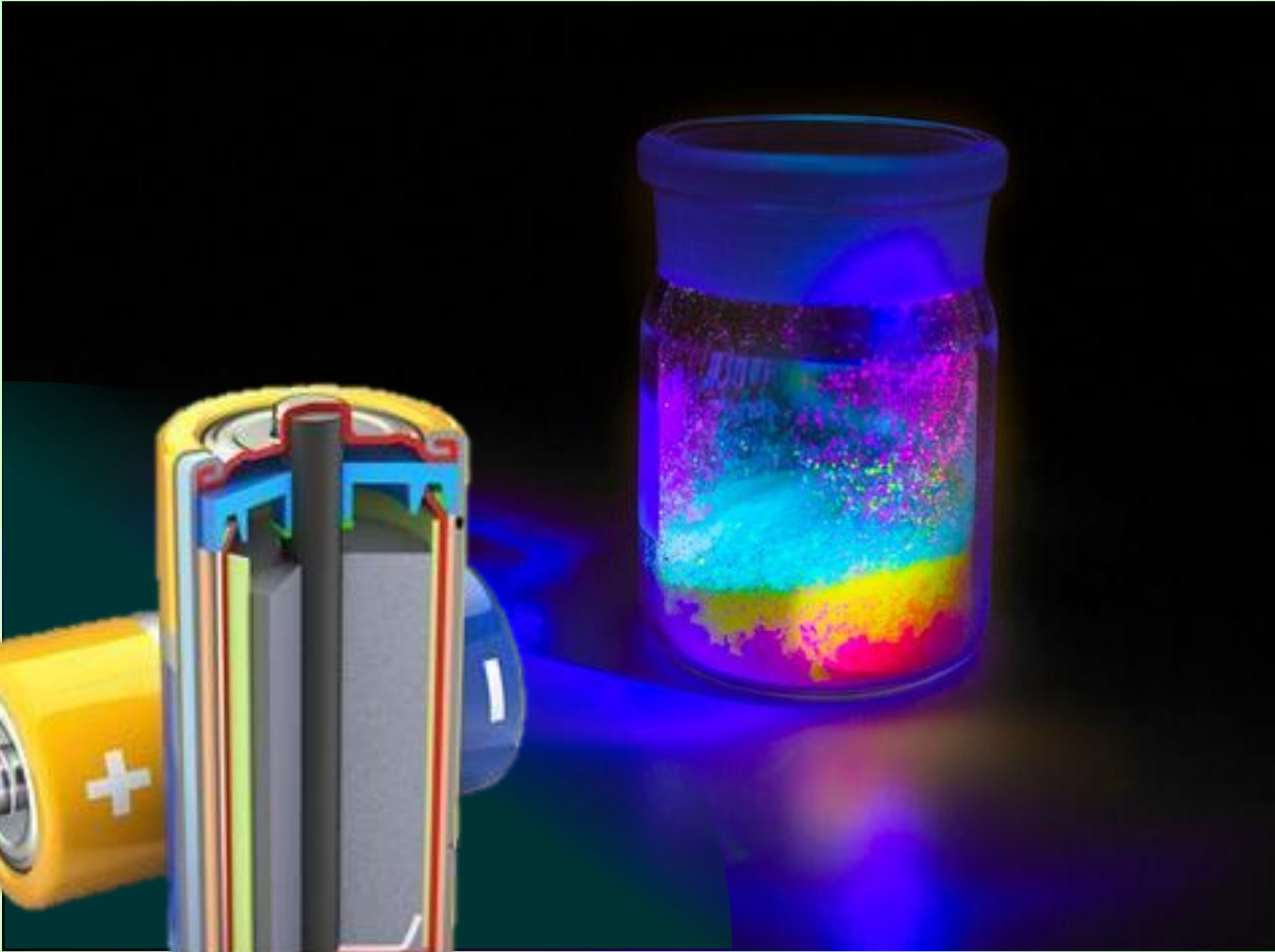
Final Workshop of the project



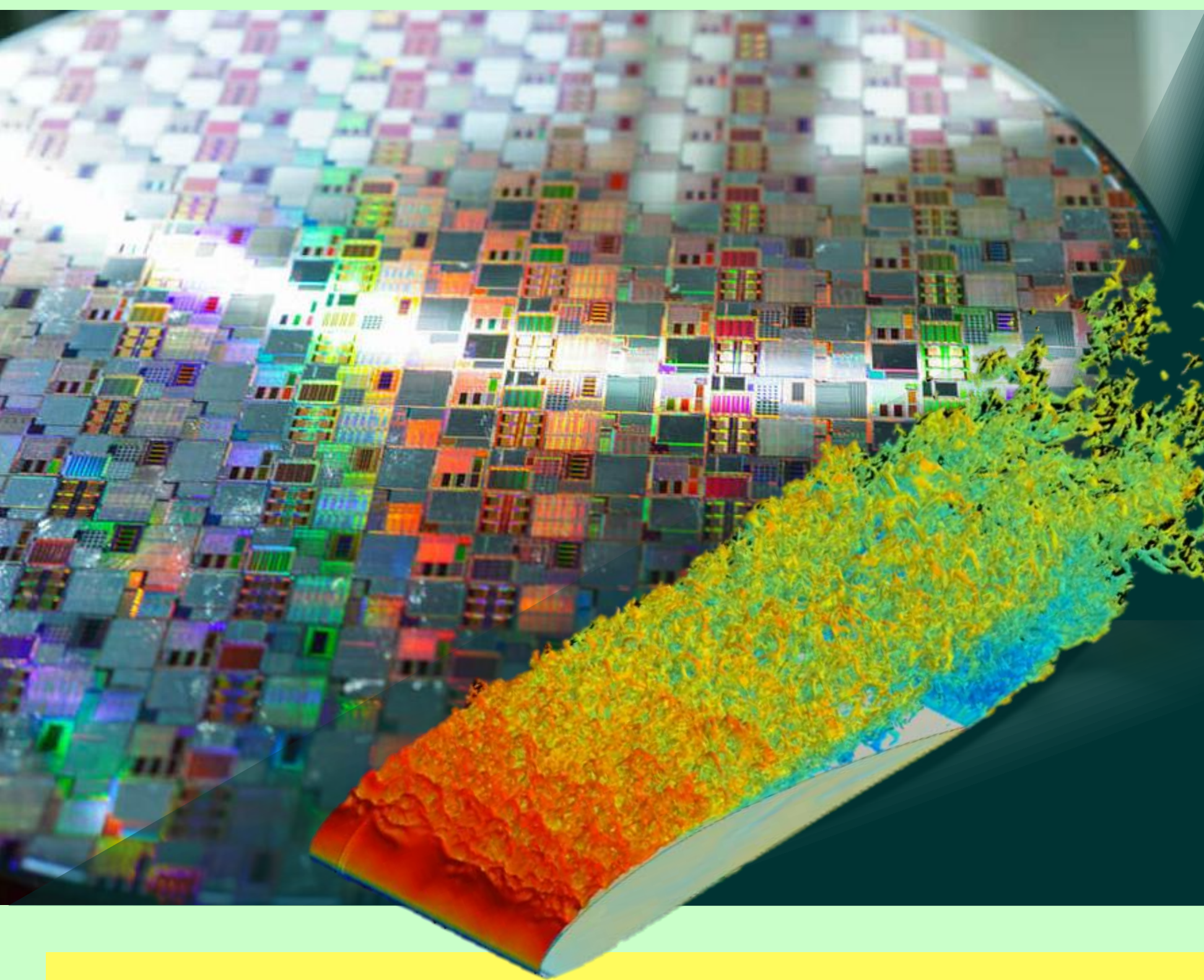
UNIMORE-Data Center, Via E. Gorrieri, 31, 41122 Modena - 30/10/2025

From 9:00 to 9:15	Welcome address and introduction to the ECOSISTER Spoke 6 goals and activities	Scientific computing and HPC for innovation: ECOSISTER Spoke 6
Speaker:	Roberto De Renzi Uni-Parma	

Time	Topic	Speaker	Title
9:15-9:45	Session Chair: Alice Ruini Keynote: Industrial / Academic Expert	Luca Larcher Applied Materials	Accelerating Material-to-Device Technology Co-Optimization Leveraging Simulation & AI
9:45-10:00	WP1: High-Throughput	Alfonso Pedone Uni-MoRe	Exploring Sodium-based Solid Electrolytes through Machine-Learning accelerated Molecular Dynamics Simulations
10:00-10:15	WP1: Green pilots	Cristina Sissa Uni-Parma	Theoretical strategies for efficient OLED materials
10:15-10:30	WP1: Response functions Spectroscopies	Pietro Bonfà Uni-MoRe	Boosting Muon Spin Spectroscopy with High-throughput Computing



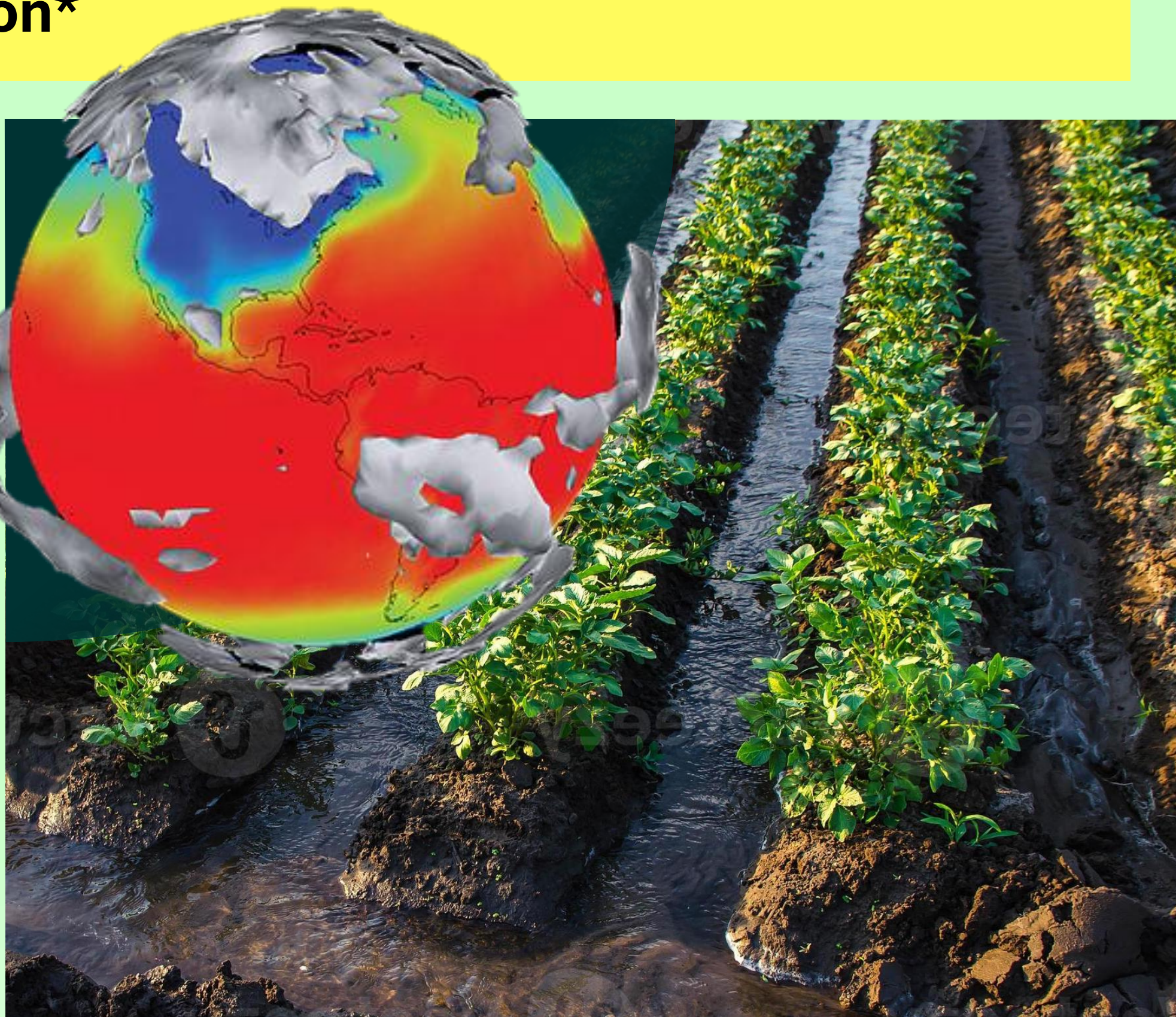
From 10:30 to 11:30	BREAK and poster session*
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Time	Topic	Speaker	Title
11:30-12:00	Session Chair: Luca Selmi Keynote: Industrial / Academic Expert	Paolo Toniutti Infineon Technologies Villach	Computational requirements in the development of electronic components
12:00-12:15	WP2: Advanced electronic and photonic components	Alessandro Ruggieri Uni-MoRe	Uprising thermal and reliability issues in advanced 3D nanoelectronics
12:15-12:30	WP2: Neuromorphic computing	Tommaso Zanotti Uni-MoRe	HPC-Enabled Design of non von Neumann Circuits for Ultra-Low Power Computing
12:30-12:45	WP2: Fluid dynamics and turbulence	Roberto Corsini Uni-MoRe	Direct numerical simulation of the separated flow around a wing section

From 12:45 to 14:15	LUNCH and poster session*
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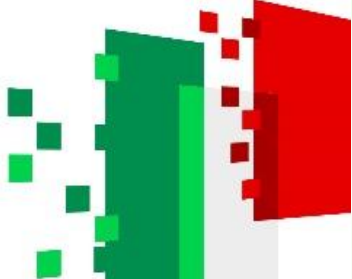
Time	Topic	Speaker	Title
14:15-14:45	Session Chair: Renato Vacondio Keynote: Industrial / Academic Expert	Günter Blöschl TU Wien and University of Bologna	Flood Hazard Mapping
14:45-15:00	WP3: Climate models	Valeria Todaro Uni-Parma	Statistical downscaling of climate model data for climate change impact assessments in the Emilia-Romagna region
15:00-15:15	WP3: Terrain analysis and surface flow propagation modeling	Riccardo Gasperoni Uni-MoRe	Lidar-Based Modeling of Riparian Tree Impacts on River Flow and Conveyance
15:15-15:30	WP3: Agriculture	Vittorio Bernuzzi and Leonardo Rossi Uni-Parma	AI-driven Aerial Vision for Sustainable Agriculture



From 15:30 to 16:30	Interactive panel on: Strengthening innovation via scientific and high-performance computing: state of play and what is next Representatives from Institutions, RTOs (Cineca, Infn), experts, stakeholders, researchers.
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* Poster session next page



Poster exhibition Spoke 6

Final Workshop of the project



0.1	ECOSISTER SPOKE 6 and its cascaded initiatives: WPs, Topics, People, and Competences	
0.2	ECOSISTER SPOKE 6 - WP1 - Advanced materials	
0.3	ECOSISTER SPOKE 6 - WP2 - Electronic, photonic and mechanical components for energy and sustainability	
0.4	ECOSISTER SPOKE 6 - WP3 - Cross-disciplinary methods, Water flow, Agriculture, and Climate	
0.5	Supporting Sustainable Scientific Simulations and Industrial Applications through HPC – CINECA activities in ECOSISTER Spoke 6 F. Affinito, A. Acocella, A. Emerson, T. Gorni, L. Bellentani, L. Querciagrossa, M. Ippolito, E. Pascolo	Cineca, Casalecchio di Reno (BO)
0.6	Infrastructure management and user support Alessandro Pascolini, Claudio Grandi, Carmelo Pellegrino	INFN

WP1 Research activities		
1.1.1	Pressure And Magnetic Field Control Of The Topological Phase In Antiferromagnetic Bilayers Narsimha Rao Elaprolu, and Marco Gibertini	Università degli Studi di Modena e Reggio Emilia
1.2.1	Molecular modeling studies on the effect of polymer-electrolyte interactions in the Li-ion batteries Michele A. Salvador, Rita Maji, Elena Degoli, Alice Ruini, and Rita Magri	Università degli Studi di Modena e Reggio Emilia
1.2.2	Photoinduced charge separation in single-component squaraine thin films: the key role of electrostatic disorder Davide Giavazzi, Anna Painelli	Università di Parma
1.2.3	Silicon based materials for energy storage applications Omar Lopez Estrada, Rita Maji, Alice Ruini, Rita Magri, Michele Salvador, Ivan Marri, Elena Degoli	Università degli Studi di Modena e Reggio Emilia
1.2.4	Carrier Multiplication in Si Nanocrystals: an ab initio Study Manaswita Kar, Marco Govoni and Ivan Marri	Università degli Studi di Modena e Reggio Emilia
1.3.1	First principles characterization of opto-electronic properties and defect engineering of emerging materials for next-generation electronics and optics Luca Bursi, Tommaso Gorni, Angela Acocella, Fabio Affinito, Alice Ruini	Università degli Studi di Modena e Reggio Emilia
1.3.2	Defect complexes and charge compensation in Ta-doped anatase TiO2 transparent conductor Luca Bursi, Alessandra Catellani, Piero Mazzolini, Cristina Mancarella, Andrea Li Bassi, Andrea Baraldi, Arrigo Calzolari	Università degli Studi di Modena e Reggio Emilia
1.3.3	First-principles study of bound excitons in monolayer SnS ₂ Vinicius Alves Bastos, Fulvio Paleari, Eleonora Luppi, Marco Gibertini, and Alice Ruini	Università degli Studi di Modena e Reggio Emilia
1.3.4	Non-adiabatic Molecular Dynamics Applied to Muons: Computation of Stopping Power Adrian Gomez Pueyo ¹ , Alberto Castro ² , Roberto De Renzi ¹ , Pietro Bonfà ³	¹ Università di Parma, ² Universidad de Zaragoza, Spain, ³ Università degli Studi di Modena e Reggio Emilia

WP2 Research activities		
2.1.1	Neural Strategies for Upper Limb Movements: Motor Unit Control during Dynamic Contractions at Increasing Speeds Mattia Orlandi ¹ , Pierangelo M. Rapa ^{1,2} , Farah Baracat ^{3,4} , Luca Benini ^{1,4} , Elisa Donati ^{3,4} , Simone Benatti ²	¹ Università di Bologna, ² Università degli Studi di Modena e Reggio Emilia, ³ University of Zurich, ⁴ ETH, Zurich
2.1.2	Application and highly efficient coupling of hollow-core fibers for wideband communication and sensing Lorenzo Rosa, Federico Melli, Luca Vincetti	Università degli Studi di Modena e Reggio Emilia
2.1.3	HPC-driven thermal design of GaN-based, highly-efficient converters for next generation photovoltaics Payam R. Kalvani, Pierpaolo Palestri, Luca Selmi	CASCADED CALL Università di Parma
2.2.1	Turbulence around a wing section in separated flow conditions Roberto Corsini, Andrea Cimarelli, Enrico Stalio	Università degli Studi di Modena e Reggio Emilia
2.2.2	Direct numerical simulation of wind-waves Marco Crialesi Esposito, Andrea Cimarelli, Enrico Stalio	Università degli Studi di Modena e Reggio Emilia
2.2.3	RANS representation of a low-Reynolds number blade section at high angles of attack Luca Pagliarini ¹ , Roberto Corsini ² , Enrico Stalio ² , Fabio Bozzoli ¹ , Sara Rainieri ¹	¹ Università di Parma, ² Università degli Studi di Modena e Reggio Emilia

WP3 Research activities		
3.0.1	Boundary-drift driven diffusion and uphill phenomena Francesco Casini, Cristian Giardinà, Jacopo Nicolini, Luca Selmi, Cecilia Vernia	Università degli Studi di Modena e Reggio Emilia
3.1.1	Forecasting biodiversity loss in agricultural ecosystems Michele Bellingeri ¹ , Davide Cassi ¹ , Davide Martinetti ² , David Bohan ² , Daniele Bevacqua ²	¹ Università di Parma, ² INRAE, Avignon, France
3.2.1	Artificial intelligence for water flow prediction from synthetic data Pietro Musoni , Alessandro Dal Palù	Università di Parma
3.2.2	Monte Carlo Evaluation of Levee Reliability Under Hydraulic Loading and Mammal Bioerosion Rachit Soni, Giovanni Moretti, Marco Redolfi, Stefano Orlandini	Università degli Studi di Modena e Reggio Emilia
3.2.3	Robust Statistical Processing of Long-Time Data Series to Estimate Soil Water Content Mirko Anello ¹ , Fabrizio Laurini ¹ , Marco Riani ¹ , Roberto Valentino ¹ , Marco Bittelli ² , Massimiliano Bordoni ² , Claudia Meisina ³	¹ Università di Parma, ² Università di Bologna, ³ Università di Pavia
3.2.4	3D SPH simulations of Bridges during flood conditions Aaron English, Susanna Dazzi, Renato Vacondio	Università di Parma
3.2.5	Investigating the migration of immiscible contaminants fluid flows in homogeneous and heterogeneous aquifers with high-resolution numerical simulations Michele Pasquali, Alessandra Feo, Fulvio Celico	Università di Parma

