



AGENDA

JAN 12	19:00 CET	Welcome reception
JAN 13	9:00 CET	Welcome and opening
	9:15 CET	<i>The global Earth System simulated at 1 km: the large-scale of small-scales</i> Daniel Klocke ♦ Max Planck Institute of Meteorology
	9:45 CET	<i>Supercomputing for Climate Extremes: Global Storm-Resolving Models and Advanced Satellite Observations</i> Masaki Satoh ♦ University of Tokyo / Yokohama National University
	10:15 CET	Q&A
	10:30 CET	<i>Digital Twin in Oncology: How Artificial Intelligence can help</i> Emmanuel Barillot ♦ Institut Curie
	11:00 CET	Coffee-break
	11:30 CET	<i>Scaling Laws in HPC and AI</i> Rio Yokota ♦ RIKEN / Tokyo Tech
	12:00 CET	Q&A
	12:15 CET	<i>Artificial Intelligence and the study of Materials for Energy</i> Núria López ♦ Instituto Catalán de Investigación Química
	12:45 CET	<i>Computational Science for Photoenergy Conversion Materials</i> Koichi Yamashita ♦ Yokohama City University
	13:15 CET	Q&A
	13:30 CET	Lunch

PLENARY ROOM

	MR1 <i>Climate Modelling</i>	MR2 <i>Biomedical Applications</i>	PR <i>Material Sciences</i>
15:00 CET	Introduction Mario Acosta ♦ Barcelona Supercomputing Center	TBC	SIESTA: Overview of features & performance A. Garcia
15:30 CET	Earth system model workflow interface Kai Keller ♦ Barcelona Supercomputing Center		Optimizing wave functions in quantum Monte Carlo M. Casula

CAPTION

MR1 MEETING ROOM 1 • MR2 MEETING ROOM 2 • PR PLENARY ROOM • SMR SMALL MEETING ROOM



AGENDA

JAN
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	MR1 <i>Climate Modelling</i>	MR2 <i>Biomedical Applications</i>	PR <i>Material Sciences</i>
15:45 CET	High Performance Climate and Weather Benchmark Joachim Biercamp ♦DKRZK	TBC	Quantum Monte Carlo for Machine-Learning N. Nakano
16:00 CET	LES modeling Piotr Dziekan ♦ University of Warsaw	TBC	Unveiling the Yambo code: Features, Performance, and Applications in Material Science D. Varsano
16:30 CET	Coffee break		
17:00 CET	The FESOM ocean model - HPC aspects Miguel Andrés-Martínez ♦ AWI	TBC	libNEGF: a general-purpose non-equilibrium Green's function library and applications A. Pecchia
17:30 CET	EDITO: an HPC perspective Stella Paronuzzi ♦ Mercator	TBC	Remote management of Interoperable Workflows on Heterogeneous supercomputers: case study on drug resistance of HIV-1 L. Genovese
17:40 CET			ChASE Eigensolver on Multi-GPUs: Algorithm, Parallelism, and TDD-Driven Refactoring X. Wu
18:00 CET			Integrating ChASE eigensolver with the Yambo code R. Richefort

CAPTION

MR1 MEETING ROOM 1 • MR2 MEETING ROOM 2 • PR PLENARY ROOM • SMR SMALL MEETING ROOM

AGENDA

JAN
14

MR1

Climate Modelling

08:00 CET	Shin-ichiro Shima ♦ University of Hyogo
08:30 CET	Fugaku and the NICAM atmospher model Hisashi Yashiro ♦ NIES

PR

Material Sciences

MR2

Biomedical Applications

09:00 CET	A workflow for NICOCO: Automation, reproducibility and provenance with Autosubmit Leo Arriola & Miguel Castrillo ♦ Barcelona Supercomputing Center	What would be the future Eigenvalue solver for Material Science? T. Imamura	Summary of WP5 José Carbonell
		Reducing Numerical Precision Requirements in Electronic Structure Calculations W. Dawson	Implementing building blocks and workflows in biomedical applications
10:00 CET	HPCW Workshop David Guibert ♦ Eviden	Radiation damage in nuclear materials E. Artacho	Benchmarking multiscale simulation tools
		A route to photophonics: from ferroelectrics to charge density waves R. Rurali	Mechanochemical subcellular- element model of crawling cells
11:00 CET	Coffee break		

11:30CET	WP4 Internal Discussion: Status and future plans	Exploration of electrochemical interfacial processes using DFT and classical liquid theory hybrid simulations M. Otani	Modelling intracellular behaviour in multiscale simulations
12:00 CET		QM/MM simulations of the electrochemical interface P. Ordejon	Integrating boolean models on cells
12:30 CET	Replicability in Earth System Models Marta Alerany ♦ Barcelona Supercomputing Center	Simulating advanced materials: new and upcoming features in SIESTA N. Wittemeier	From molecular dynamics to logical rules in intracellular models
13:00 CET	Amanda Duarte ♦ Barcelona Supercomputing Center	Electronic and Optical Features of Pb- less and Pb-free 2D and quasi-2D halide perovskites G. Giorgi	Final conclusions on the Biomedical applications project

13:30 CET	Lunch
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MR1 MEETING ROOM 1 • **MR2** MEETING ROOM 2 • **PR** PLENARY ROOM • **SMR** SMALL MEETING ROOM



AGENDA

JAN
14

	MR1 <i>Climate Modelling</i>	PR <i>Material Sciences</i>
15:00 CET	Reconstruction and downscaling of historical land surface boundary conditions with Machine Learning Amirpasha Mozaffari ♦ Barcelona Supercomputing Center	Defects and grain boundary structure of lead-free perovskites K. Yamashita Unravelling the charge transfer mechanism in ZnWO ₄ :Yb ³⁺ :Cr ³⁺ for upconverted luminescence C. Borghesi
15:30 CET	Wrap up and conclusions	Investigating phase diagram and phonons in superconducting Lanthanum Hydride using ab-initio methods accelerated by machine learning potentials A. Raghav
16:00 CET		Phase diagram of superconductive sulfur hydride and its anharmonic phonons M. Cherubini
16:30 CET	Coffee break	
17:00 CET	Funding opportunities (WP4, WP5 & WP6) PR	

CAPTION

MR1 MEETING ROOM 1 • **MR2** MEETING ROOM 2 • **PR** PLENARY ROOM • **SMR** SMALL MEETING ROOM



AGENDA

JAN 15	9:00 CET	Introduction to final plenary
	9:15 CET	WP4 Conclusions
	9:30 CET	WP5 Conclusions
	9:45 CET	WP6 Conclusions
	10:00 CET	<i>The Convergence and Divergence of HPC and AI</i> Mohamad Wahib ♦ RIKEN Center for Computational Science (<i>online</i>)
	10:30 CET	<i>The impact of AI in Biomedicine</i> Alfonso Valencia ♦ Barcelona Supercomputing Center
	11:00 CET	Q&A
	11:15 CET	Coffee-break
	11:45 CET	<i>The Digital Revolution of Earth System Modelling</i> Peter Dueben ♦ European Centre for Medium-Range Weather Forecasts (<i>online</i>)
	12:15 CET	<i>Spin-orbit torque in two-dimensional materials as a platform for efficient and non-volatile memories</i> José Hugo García ♦ Catalan Institute of Nanoscience and Nanotechnology
	12:45 CET	Q&A
	13:00 CET	Lunch
	15:00 CET	HANAMI General Assembly

PLENARY ROOM