HANAMI
EU-Japan Alliance in HPC

AGENDA

JAN 12

19:00 CET	Welcome reception

JAN 13

PLENARY ROOM

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

	MR1 *Climate Modelling*	**MR2** *Biomedical Applications*	**PR** *Material Sciences*
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

Funded by the European Union
EuroHPC Joint Undertaking

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		MR1 *Climate Modelling*	MR2 *Biomedical Applications*	PR *Material Sciences*
JAN 13	15:45 CET	**High Perfomance 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

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JAN 14

	MR1 *Climate Modelling*	PR *Material Sciences*	MR2 *Biomedical Applications*
08:00 CET	Shin-ichiro Shima ✦ University of Hyogo		
08:30 CET	**Fugaku and the NICAM atmospher model** Hisashi Yashiro ✦ NIES		
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 photophononics: 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	**SElectronic and Optical Features of Pb-less and Pb-free 2D and quasi-2D halide perovskites** N. Wittemeier	**Final conclusions on the Biomedical applications project**
13:30 CET	**Lunch**		

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	MR1 *Climate Modelling*	PR *Material Sciences*
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 ZnWO4:Yb3+: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 anahrmonic phonons** M. Cherubini
16:30 CET	**Coffee break**	
17:00 CET	**Funding opportunities (WP4, WP5 & WP6)** **PR**	

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PLENARY ROOM

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

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