

EuroHPC Summit Week 2020

Tuesday 24 March 2020

Computational Materials Science towards the Exascale: performance portability and use cases - Cavado (14:30-16:00)

-Conveners: Ivan Marri; Maria Celeste Maschio; Andrea Ferretti; Elisa Molinari

time	[id] title	presenter
14:30	[86] Co-designing and porting MaX codes to ARM SVE and heterogeneous architecture	CAVAZZONI, Carlo
14:55	[87] Software engineering towards exascale: domain specific libraries, communication optimality, and machine learning	VANDEVONDELE, Joost
15:20	[88] Performance portability of GW and many-body perturbation theory codes: the case of Yambo on GPUs	SPALLANZANI, Nicola
15:40	[93] Parallelization and optimization of the FLEUR code: new possibilities for all-electron Density Functional Theory	ALEKSEEVA, Uliana

Computational Materials Science towards the Exascale: performance portability and use cases - Cavado (16:30-18:10)

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time	[id] title	presenter
16:30	[89] High-throughput computational discovery and characterization of novel low-dimensional materials for applications in energy and electronics	CAMPI, Davide
17:00	[90] Addressing electrified water-metal interfaces at the atomic level with TranSIESTA	ORDEJÓN, Pablo
17:30	[92] Organic-metal interfaces studied using DFT and GW ab initio methods with Quantum ESPRESSO and Yambo	CARDOSO, Claudia