

MAX3: MAterials design at the eXascale

Description

Understanding, predicting, and discovering the properties and performance of materials is key to delivering the technologies that power our economy and allow for the sustainable development of our society. For this reason, materials simulations have become one of the most intensive and fast growing domains for high-performance computing worldwide, with a recognized European leadership in developing and innovating the ecosystem of quantum simulation codes.

MaX will target these lighthouse codes to address these challenges and leverage the opportunities arising from future exascale and post-exascale architectures and offer powerful paths to discovery and innovation, serving both scientific and industrial applications. MaX includes (1) the core developing teams of the European lighthouse codes; (2) the HPC centres designing and hosting preexascale and exascale systems; (3) the main European companies engaged in the development of exascale technologies; and it brings (4) a sustained record in training and educating the community, and (5) in disseminating its resources under an extensive open source model that includes codes, workflows, and FAIR data.

These synergies will underpin the objectives of the project, which aim to upscale the MaX codes and their performance on multiple heterogeneous exascale architectures; to endow these codes with innovative capabilities enabled by such architectures; to co-design the hardware and software in collaboration with the relevant European stakeholders; to enable turn-key simulation capabilities that meet the power of exascale resources and deliver the resilience needed; to disseminate the entire ecosystem of codes, workflows, and data; and to train and engage developers and users in fully leveraging such powerful instruments for discovery and innovation.

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