

[Inici](#) > MAX: MAterials design at the eXascale. European Centre of Excellence in materials modelling, simulations,

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Description

The main goal of MaX is to allow the pre-exascale and exascale computers expected in Europe in the 2020s to meet the demands of a large and growing base of researchers committed to materials discovery and design. This goal will be achieved through:

- an innovative software development model, based on the concept of separation of concerns, that will enable performance of the community codes on heterogeneous hardware architectures, without disrupting their internal structure, the richness of their simulation capabilities, and their distributed and open development model. In this way, the most important community codes for quantum mechanical materials modelling will be ready for pre-exascale machines by the completion of the MaX programme, and prepared to be ported to new architectures as they will become available;
- an integrated ecosystem enabling the convergence of high performance and high throughput computing, that will allow for the steering of the millions to hundreds of millions of simulations that are needed to optimise the properties and performances of a material or a device, with robust and reproducible workflows, all contributing to an ever growing repository of curated data;
- a new approach to scientific computing in which hardware and software are co-designed and co-developed taking into account mutual constraints and goals;
- innovative measures for easy access to materials science applications, for engaging academic and industrial communities and fostering a broader and diverse pool of well trained users and developers.

All this is made possible by the coordinated effort of a team involving developers of the leading EU open source community codes in the materials domain, five leading European HPC centres, two technology partners, and training and communication experts. MaX is fully aligned with the long term European HPC strategy and community, and to the work program call INFRAEDI-02-2018 Subtopic (a), area 5.

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

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