

MaX: MAterials design at the eXascale

Description

Materials are crucial for scientific and technological advances, industrial competitiveness and for tackling key societal challenges - from energy and environment to health care, information and communications, manufacturing, safety and transportation. The current accuracy and predictive power of materials' simulations allows a paradigm shift for computational design and discovery, in which massive computing efforts can be launched to identify novel materials with improved properties and performance; to address behaviours of ever-increasing complexity; to accelerate synergies and sharing data and work-flows and to empower the science of big-data; and to provide services in the form of data, codes, expertise, turnkey solutions, and a liquid market of computational resources.

Europe has the human resources, track record and infrastructure to be a worldwide leader in this field, and we want to create a CoE in materials' modelling, simulations, and design to endow our researchers and innovators with powerful new instruments to address the key scientific, industrial and societal challenges that require novel materials. This CoE will be a user-focused, thematic effort supporting the needs and the vision of all our core communities: domain scientists, software scientists and vendors, end-users in industry and in academic research, and high-performance computing centres. The proposal is structured along two core actions:

- Community codes, their capabilities and reliability; provenance, preservation and sharing of data and work-flows; the ecosystem that integrates capabilities; and hardware support and transition to exascale architectures.
- Integrating, training, and providing services to our core communities, while developing and implementing a model for sustainability, with the core benefit of propelling materials simulations in the practice of scientific research and industrial innovation.

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