MAX

The **MAX Centre of Excellence** is a partnership of European leaders in the domain of computational materials research, European HPC centres, technology partners, and code developers.

Proudly co-f nanced by the EuroHPC Joint Undertaking for the 2023-2026 period, MAX started in 2015 and has been successful in three consecutive editions since then.

MAX's current challenge lies in redesigning the most used open-source community codes in quantum materials simulations and the related data ecosystem to take full advantage of the exascale technology. By developing and optimizing energy-ef cient computing tools, MAX provides an environmentally sustainable way of doing science.

Where to f nd us

www.max-centre.eu

@max_center2

/company/max-centre

@MaXCentreeXascale

Co-Funded by the European Union

MAX - MAterials design at the EXascale has received funding from the European High Performance Computing Joint Undertaking under grant agreement no. 101093374 and from national agencies from participating countries (Czechia, France, Germany, Italy, Slovenia, and Spain).

EuroHPC Joint Undertaking

Views and opinions expressed are however those of the author(s) only and do not necessarily ref ect those of the European High Performance Computing Joint Undertaking. Neither the European Union nor the granting authority can be held responsible for them.

MAX DRIVING THE EXASCALE TRANSITION

MAX – MAterials design at the eXascale

MAX is a European Centre of Excellence that enables materials modelling, simulations, discovery, and design at the frontiers of the current High-Performance Computing (HPC), promoting the use of exascale and post-exascale computing capabilities.

DRIVING THE EXASCALE TRANSITION

Materials research in the eXascale era

Exascale computing (10^{18} operations per second) is disrupting the capability of computer simulations and data processing, with tremendous consequences in all scientif c f elds, including materials science as a clear-cut use case. Yet, the road towards exascale technology is f lled with challenges:

Design new paradigms for developing, managing, and deploying software and workf ows that fully exploit the exascale architecture.

Enable the scalability and ef ciency of the scientif c codes in a reliable and resilient infrastructure, leveraging on state-of-the art accelerators, networks, and storage systems.

Investigate methods to develop power-ef cient software and decrease energy consumption by using European Energy Aware Runtime systems.

Impacts

The most broadly used open-source codes for quantum simulations in materials are ported and scaled on multiple new and heterogeneous computing architectures, while optimised in terms of energy ef - ciency.

Exchange of information and expertise among software and HPC hardware de-velopers is facilitated to guarantee that new software adapts to future computer architectures and, conversely, new power-ful hardware meets the needs of materials scientists.

Training and education programs are of ered to software end-users and developers in the materials domain, in coordination with actors in the EuroHPC and European ecosystem. MAX hands-on courses are designed to enable the best understanding and use of codes, workf ows, and turnkey solutions, fostering a community of advanced developers.

EXascale workf ows and extreme data handling are designed and deployed to empower users in materials simulations to tackle key scientif c challenges in materials science.