DRIVING THE EXASCALE TRANSITION

The revolution of the exascale computing (10^{18} operations per second) will disrupt the capability of computer simulations and data processing. It will have consequences in all scientific fields, from **nuclear physics** to **climatology** to **materials science.**

The road towards exascale technology sets a large number of challenges. **Software**: new development models. **Hardware**: new architectures and the overcome of miniaturisation limits. **Environment**: power consumption of computers, and many others.

MAX - MAterials Design at the eXascale

MAX is a European Centre of Excellence which enables materials modelling, simulations, discovery and design at the frontiers of the current and future **High Performance Computing** (HPC), **High Throughput Computing** (HTC) and **data analytics technologies**.

MAX challenge lies in redesigning the most used **open source codes** in quantum **materials simulations** and the related data ecosystem in order to take advantage of the exascale technology.

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Join the MAX community!
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MAX DRIVING THE EXASCALE TRANSITION

IMPACTS

- Bring the most successful and widely used open-source, community codes in quantum simulations of materials towards exascale and extreme scaling performance
- Co-design activities to ensure that future HPC architectures are well suited for materials domain applications and viceversa
- Enable the convergence of high-performance and high-throughput computing with high-performance data analytics in the materials domain
- Widen the access to codes, provide workflows and turn-key solutions to empower user communities in materials simulations
- Foster the engagement and know-how of users communities in industry and academia

NETWORK

MAX CoE is a partnership of European leaders in the materials domain, prominent European HPC centres, technology partners and training & communication experts.

EUROPEAN CENTRE OF EXCELLENCE FOR MATERIALS DESIGN

TIER 0 HPC CENTRES	CODES & ECOSYSTEM DEVELOPERS	TECHNOLOGY PARTNERS	COMMUNICATION, TRAINING & DISSEMINATION
CINECA	Consiglio Nazionale delle Ricerche	arm	UNESCO
JÜLICH Forschungszentrum	QUANTUM ESPRESSO	E4 COMPUTER ENGINEERING	cecam
Barcelona Supercomputing Center	SISSA		Psi-k
cea	Yambo		GHENT UNIVERSITY
ETH zürich	siesta		Trust-IT Services
	ICN2		
	JÜLICH Forschungszentrum		
	fleur		
	CP2K		
	ETH zürich		
	cea		
	big DFT		
	EPFL		
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MAX coordination and management: Cnr - Modena, Italy

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