### European Centre of Excellence



### **DRIVING THE EXASCALE TRANSITION**

Enabling materials modelling, simulations, and design at the frontiers of current High-Performance Computing

### Meet the MaX Consortium



MAX COORDINATION AND MANAGEMENT: CNR - MODENA, ITALY

## Impact of MaX lighthouse codes on European research



#### 2024 European Distribution of Authors' Affiliation in Peer-reviewed Publications

#### explore the MaX codes

MaX open-source materials simulation codes are adopted by a large number of research and industry end-users, both across Europe and worldwide, to address scientific grand challenges via exascale workflows and extreme data.

In 2024, MaX codes received 4081 citations, 1858 of which from European affiliations.

## **Deployments and benchmarks** on EuroHPC architectures



MaX codes are deployed on many EuroHPC machines with modules available to users (M), or demonstrated by the developers and ready for installation (D). Code benchmarks (B) are available on MaX GitLab repo. Almost all architectures are supported (S) and ready for automatic deployment.



# **Performance & Scalability of** MaX lighthouse codes



download the

brochure

MaX codes can exploit the computational power expressed by NVIDIA and AMD GPUs to achieve high parallel efficiency on different EuroHPC architectures:

Comparison of a middle-sized DURNTUMESPRESSO benchmark system on different parallel systems: 300 calls isdy 200 edup GPU 24 for (sec) 100 CPU BASIC FFTs BATCHED BATCHED MPI-GPU





Parallelization over independent kqleur points and scaling of single kq-point over multiple GPUs (4 per node) NaCl 10 k-points



## **Energy savings of MaX codes on** various HW platforms



Measured and optimized with MERIC, using simple static scaling of CPU and GPU power management knobs.





### **MaX Training Programs**

visit our agenda



12	3934	31	15
trainings, schools, and hackathons	professionals trained	hosted researchers for tailored training	collaborations with NCCs and CoEs
	in the first	2 years of activity	

MaX web: https://www.max-centre.eu/



MaX Newsletter: https://bit.ly/MaXCoENewsletter

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