European Centre of Excellence

MaX

DRIVING THE EXASCALE TRANSITION

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

Meet the MaX Consortium

Energy savings of MaX codes on various HW platforms

https://bit.ly/max-energy-consumption-report

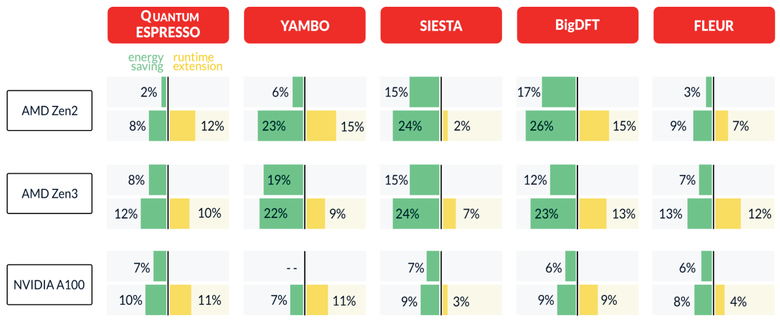
To enhance efficiency in MaX codes, static tuning of hardware power knobs was applied on selected platforms. Energy efficiency is measured as average FLOPs per Watt of power, where FLOPs are obtained through platform-specific performance counters over the full application run, while energy consumption is reported for the entire compute node to ensure fair comparison.

The most energy-efficient platform in our study is Intel Sapphire Rapids with HBM memory:

Quantum ESPRESSO	YAMBO	SIESTA	BigDFT	FLEUR
SPR + HBM = 4.56	SPR + HBM = 1.33	SPR + HBM = 2.57	SPR + HBM = 0.28	SPR + HBM AMD Zen2 = 1.82

Energy efficiency (FLOPs/W) on Intel Sapphire Rapids with HBM memory (and AMD Zen2 for FLEUR) and without runtime extension after the static tuning.

Since many EuroHPC systems are equipped with AMD Zen2/Zen3 CPUs and NVIDIA A100 GPUs, we chose these architectures for our tests. Energy savings were obtained by setting CPU frequencies before application execution (static tuning):



Energy consumption reduction (%) [kJ] per runtime [s]. The first row refers to a static tuning without runtime extension, while the second row reports results with maximum energy savings.

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

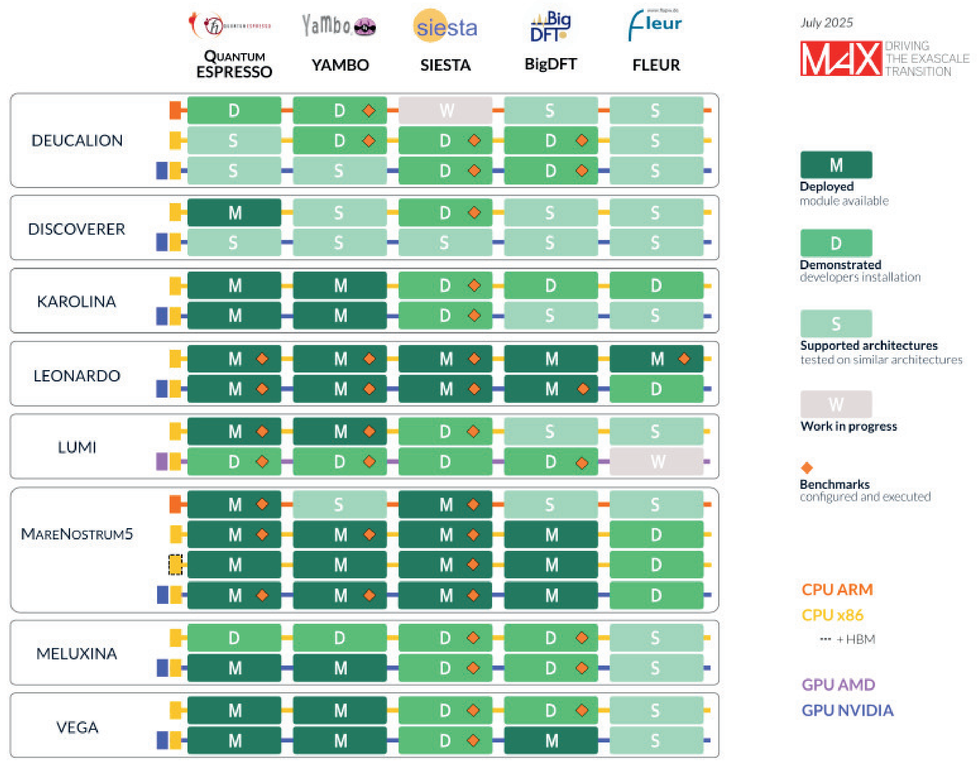
MaX Newsletter https://bit.ly/MaXCoENewsletter

Follow us on:

Deployments and benchmarks on EuroHPC architectures

https://www.max-centre.eu/exascale

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 software

https://www.max-centre.eu/software

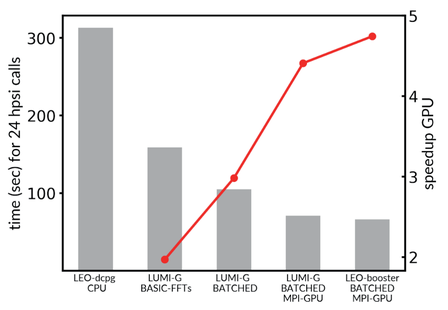
MaX develops and optimises materials science software by implementing state-of-the-art algorithms for quantum mechanical materials simulations based on density functional theory and many-body perturbation theory. Our lighthouse codes can exploit the computational power of NVIDIA and AMD GPUs to achieve high parallel efficiency on different EuroHPC architectures.

Explore the main features of the MaX lighthouse codes and compare their performance and scalability on different types of EuroHPC architectures:

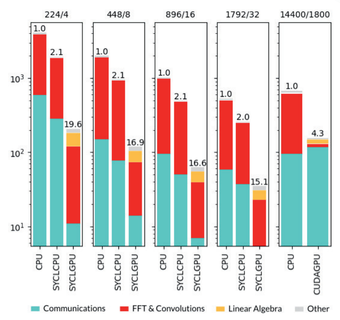
download the brochure

Performance and scalability results latest update: October 2024.

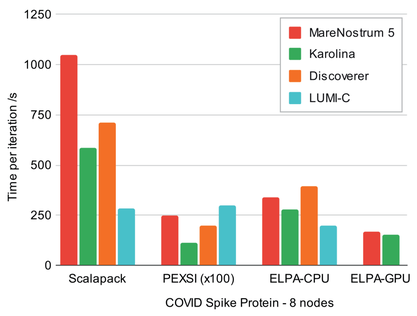
Comparison of a middle-sized benchmark system on different parallel systems:



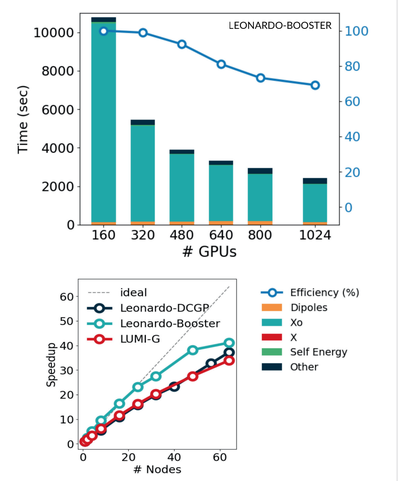
Code acceleration thanks to SYCL and CUDA programming paradigms of UO2 bulk systems:



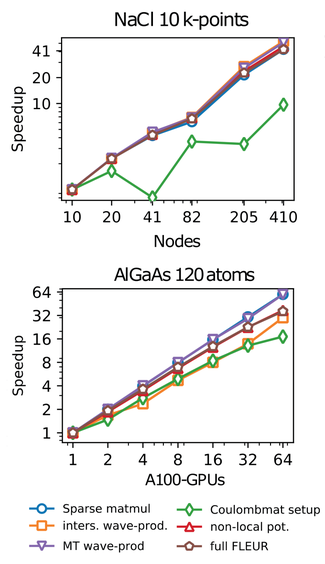
Time per solver step on different machines for a system consisting of a COVID protein in water:



Quasi-particle corrections for a GrCo interface. Scalability and speedup:



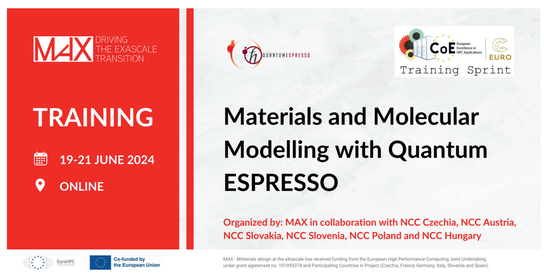
Parallelization over independent kq-points and scaling of single kq-point over multiple GPUs (4 per node):

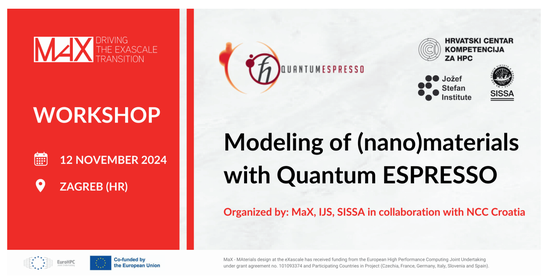


MaX Training Programs

https://www.max-centre.eu/training-events

Our training program focuses on HPC developments and computational materials science. It offers hands-on workshops, hackathons, university lectures, and tailored sessions for industrial users. Participants can also train through research projects in the MaX labs. **Several courses have been organized in partnership with the European NCCs**, and many online classes and video lectures are available to support distance learning in universities.





First 2 years of activity

12
trainings, schools, and hackathons

15
collaborations with NCCs and CoEs

3934
professionals trained

31
hosted researchers for tailored training

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