MaX - MAterials design at the eXascale

MaX (MAterials design at the eXascale) 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.

Mission

MaX aims to empower developers and users in the European **materials simulation** community to navigate the impact of massively **parallel heterogeneous computing systems**.

Drawing on the successes of its earlier phases, today the project focuses on **porting, maintaining, and scaling up advanced computer codes to the exascale level**.

This includes **turning MaX flagship codes into lighthouse applications** running on thousands of accelerated nodes and facilitating their collaborative **integration within tightly bound exascale workflows**. MaX's co-design efforts contribute to developing a strong European technology and ecosystem.

Objectives

1 Port and optimise lighthouse codes

Turn community codes for quantum materials modelling into lighthouse applications ready to run on new HPC exascale platforms while further developing their scientific capabilities.

2 Design exascale workflow and data

Design performant workflows to exploit HPC capabilities at the exascale, allow lighthouse applications to be driven automatically, and ensure the full dissemination of the entire simulation protocol, results, and data.

3 Overcome technical challenges

Identify and address the technical challenges faced by the flagship codes on their way to the exascale while providing technology insight and solutions to the code developers.

4 Leverage heterogeneous architectures

Monitor hardware and software innovations to fully exploit heterogeneous architectures while delivering validated co-design vehicles and best practices to be shared with other HPC stakeholders. Investigate methods to decrease energy consumption by using European energy aware runtime systems.

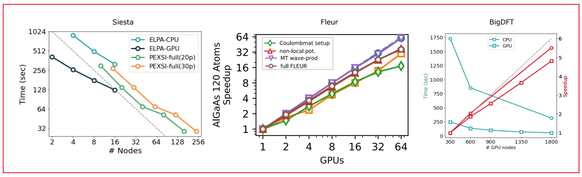
Structure

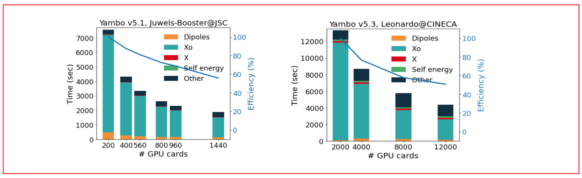
MAX CoE is a partnership of European leaders in the materials domain, prominent European HPC centres, technology partners and training & communication experts.

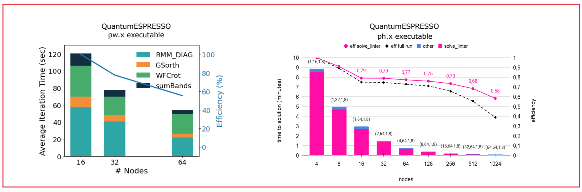
Achievements

1. Port and optimise lighthouse codes

- **Restructured and demonstrated** DeviceXlib (MaX library for performance portability) on NVIDIA, AMD, and INTEL GPU-accelerated architectures.
- **Ported** MaX codes on NVIDIA GPUs and accelerated architectures based on AMD and INTEL GPUs.
- **Equipped** codes with new features (e.g., scientific capabilities, performance and robustness algorithms).
- **Benchmarked** parallel performance of all codes and identified improvements, with special emphasis on GPU-accelerated machines. Achieved a milestone single run on the 90% of the Leonardo machine (12000 A100 next GPUs, 3000 nodes) by the Yambo code.







2. Design exascale workflow and data

- **Identified** code interoperability requirements.
- **Developed and adapted** technical tools for workflow implementation such as the AiiDA orchestrator and the HyperQueue meta-scheduler.
- **Identified and field tested** software tools to encode complex workflows.
- Concerning FAIR data and storage, **implemented** mirroring mechanism to make data stored at CSCS also available from CINECA (and soon from the Julich supercomputer centre).

3. Overcome technical challenges

- **Benchmarked and profiled** MaX codes on the GPU-accelerated EuroHPC machine Leonardo, using the JUBE software.
- **Deployed** MaX codes on EuroHPC machines, focusing on all inequivalent technologies adopted.
- Jointly with CASTIEL, **designed** a procedure for continuous integration/continuous deployment of MaX codes on EuroHPC machines.

4. Leverage heterogeneous architectures

- **Built** MaX codes on Amazon Graviton 3 (Neoverse V1) platforms (relevant for Rhea and EUPEX) with SVE vectorization activated, using multiple compilers to detect issues and provide feedback to developers.
- **Compiled** list of relevant advanced architectures available within the consortium. Performed preliminary tests with MaX codes.
- **Benchmarked** Quantum ESPRESSO, Yambo, and Siesta, and evaluated energy efficiency on two production systems at IT4I (the Barbora system and EuroHPC machine Karolina).
- **Achieved** a gain on energy to solution without compromising time-to-solution on the EuroHPC Karolina system. In particular, saved 6% (Yambo) and 16% (Siesta) of CPU energy without impacting the performance of the code by tuning the CPU core frequency.

MAX DRIVING THE EXASCALE TRANSITION
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