MAX

DRIVING THE EXASCALE TRANSITION

MAX - MAterials design at the eXascale is a European Centre of Excellence enabling materials research at the frontiers of HPC.

It involves scientists and developers of some leading electronic structure codes (including Quantum ESPRESSO, Siesta, CP2K, Yambo, Fleur, BigDFT) and HPC experts to ensure:

1 Code porting and performance on multiple and heterogeneous (GPU) HPC architectures;

2 Their integration in practical workflows to calculate advanced properties and address exascale and extreme data challenges;

3 Co-design activities focused on energy efficiency and exploitation of advanced hardware;

4 New code capabilities enabled by the HPC evolution;

5 Community hands-on training and education.

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MAX flagship codes

siesta™   CP2K   AiiDA

QUANTUM ESPRESSO   Big DFT   www.flapw.de Fleur   Yambo©

MAX partners

Electronic structure code developers and lead users experts from HPC Centres and technology companies community and education partners.

EUROPEAN CENTRE OF EXCELLENCE FOR MATERIALS DESIGN

TIER 0 HPC CENTRES	ECOSYSTEM DEVELOPERS	TECHNOLOGY PARTNERS	COMMUNICATION, TRAINING & DISSEMINATION
CINECA JÜLICH Forschungszentrum	SISSA CEA EPFL	arm E4 COMPUTER ENGINEERING	Psi-k UNESCO United Nations Educational, Scientific and Cultural Organization
BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación CEA	Consiglio Nazionale delle Ricerche ICN2 Institut Català de Nanociència i Nanotecnologia EXCELENCIA SEVERO OCHOA		CECAM Centre Européen de Calcul Atomique et Moléculaire GHENT UNIVERSITY
ETH zürich	JÜLICH Forschungszentrum ETH zürich		Trust-IT Services communicating to markets

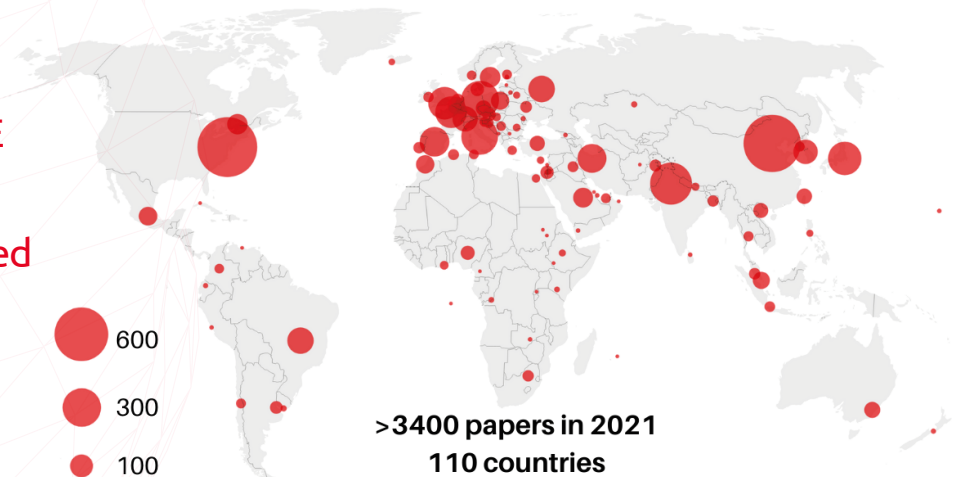**MAX is coordinated by Cnr & Unimore, Modena, Italy**

MAX Facts and Figures

130+ People involved in the CoE

100+ Events/ talks given or participated

94 Publications

**2000+** Followers in social media

600
300
100

>3400 papers in 2021
110 countries

Geographical distribution per country of scientific papers acknowledging the usage of MAX codes 2021.

Codes

- Ported on multiple homogeneous and heterogeneous (GPU) HPC architectures
- Improved performance and scaling
- Modularization, maintenance, releases, libraries
- New scientific features and algorithms developed, implemented, and released
- A detailed description can be found here: **www.max-centre.eu/software**
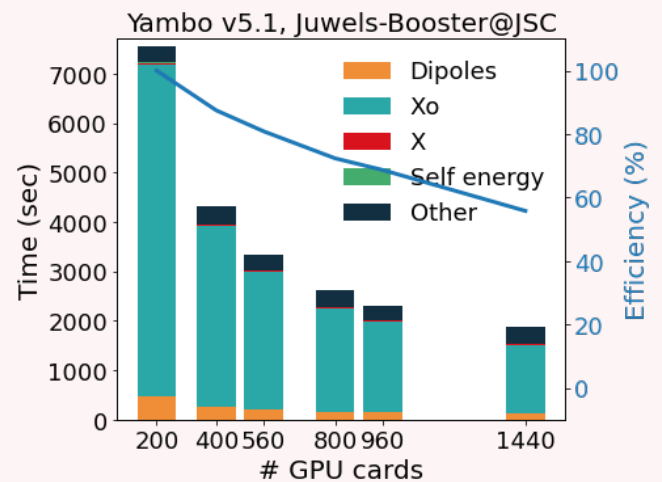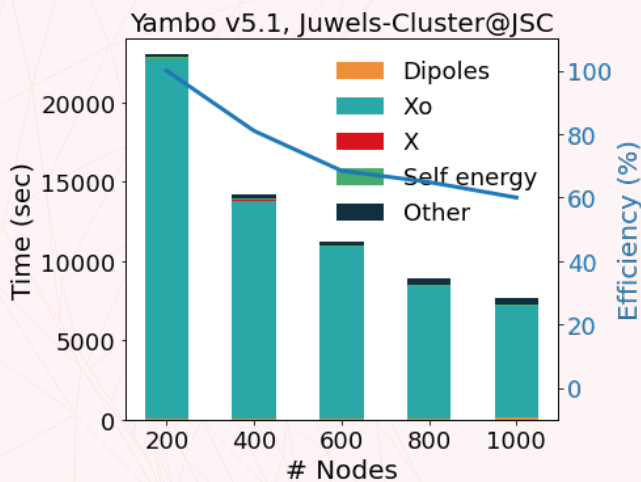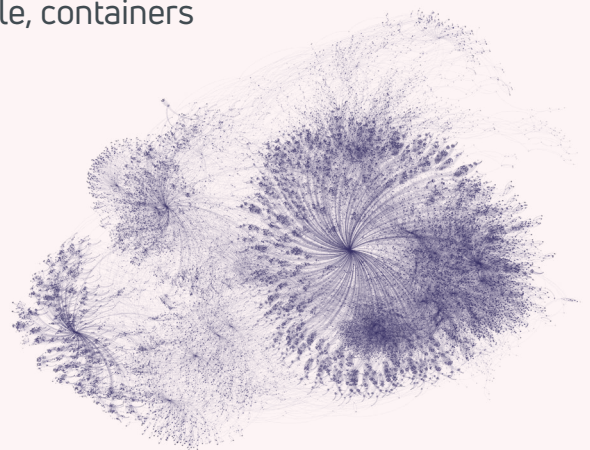

Data

- Robust automated workflows devised, developed, implemented (AiiDA based) for a number of complex materials properties
- Repository of curated data developed and made available via Materials Cloud
- Enhanced accessibility tools: AiiDAlab, Quantum Mobile, containers
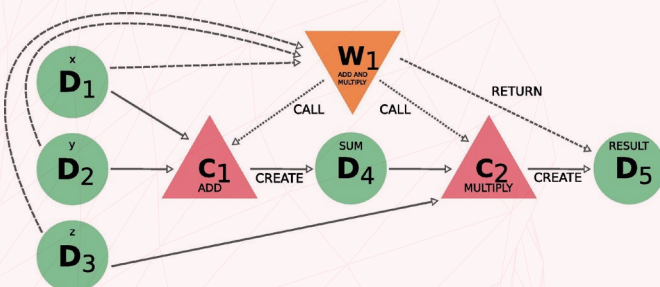
The provenance graph that is automatically generated by executing two calculation functions in succession (within an AiiDA workchain).

Connectivity of very large data sets managed by AiiDA.

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Preparing the future HPC ecosystem for electronic structure codes ("co-design")

- HW-oriented: MAX codes deployed and used as co-design vehicles on a number of advanced HW architectures (incl. ARM, AMD, NVIDIA, Intel)
- System-oriented: HPC schedulers tested using MAX workflows
- SW-oriented: middleware and HPC SW tools tested and adopted

Training and services

- Hands-on schools on MAX codes and electronic structure methods
- Rich training material developed and available online
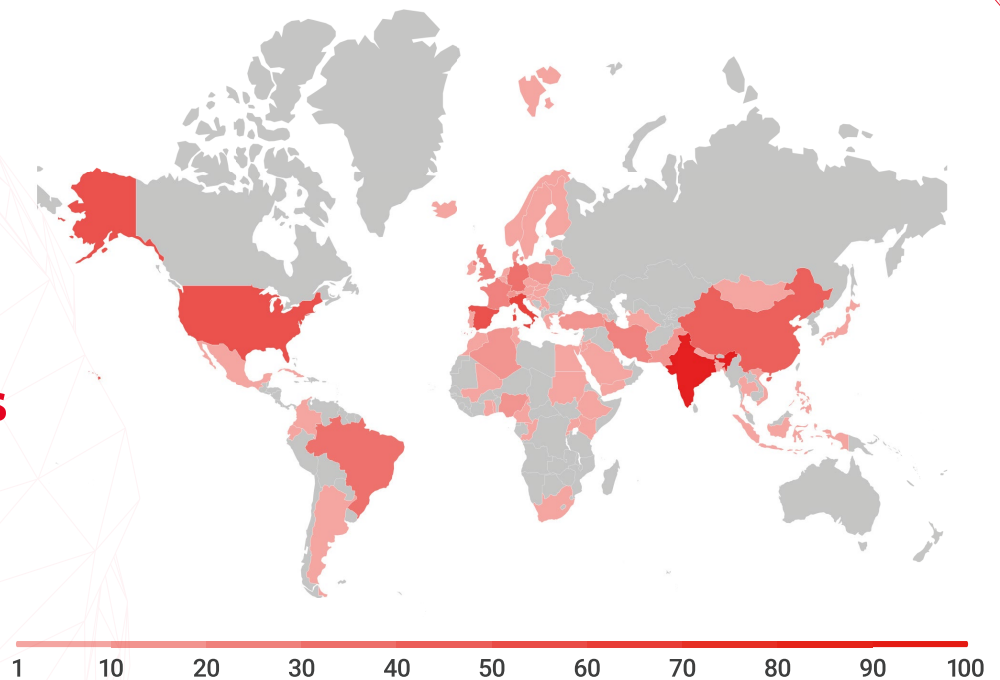- MAX coding hackathons
- Advanced support actions

8 Online Events

825 Participants

345 Lecture hours

121 Tutors

96 Lecturers

| 1 | 10 | 20 | 30 | 40 | 50 | 60 | 70 | 80 | 90 | 100 |

Global numbers of MAX training 2021 www.max-centre.eu/max-training-booklet

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MAX **Join our community!**   www.max-centre.eu   info@max-centre.eu   @max_center2