



Deliverable D10.6
Final report on MAX in the European, national,
international HPC ecosystems

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Executive Summary

This “Final report on MAX in the European, national, international HPC ecosystems” offers an overview of the activity of MAX European Centre of Excellence (CoE) as an actor of the HPC European and international ecosystem at different levels. All the activities are aimed at addressing technical and policy issues of pan-European relevance, promoting synergies and helping to overcome the fragmentation of European HPC activities on applications.

This report focuses on the period June 2020 - September 2022, and first describes MAX interactions and joint initiatives with the main European HPC actors, especially the CoEs ecosystem –including the other CoEs and their coordination instruments HPC3 and FocusCoE–, and the EuroHPC Joint Undertaking as a whole, as well as the main European organisations and projects in the field of HPC infrastructures, data and technologies –including EOSC, ETP4HPC, EPI, and PRACE–. Beside general coordination actions, we held dedicated meetings with representatives of the relevant HPC Consortia in order to best take advantage of the new EuroHPC supercomputers –especially the pre-exascale machines– since their very beginning.

MAX plays a leading role in its specific domain of materials research, and has strengthened its long-established collaboration with the relevant stakeholders. We report on the activities with the Psi-K network, CECAM, EMMC, the Battery2030+ and BIG-MAP initiatives, OptiMaDe, as well as some other relevant initiatives at national and international level.

The richness of these interactions has required significant effort from the management and all MAX partners. We believe that this investment has contributed to a more coherent, effective and friendly ecosystem in Europe, and to positioning MAX at the front of the European and global landscape in the HPC materials research.



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1. Introduction

The second half of MAX life has witnessed major advances in the European HPC and data ecosystem, with a strong increase in investments and the consolidation of the EuroHPC Joint Undertaking as a key actor. Together with Infrastructures and Technologies, Applications represent a major pillar in its strategic agenda, and Centres of Excellence (CoEs) are recognized as the key to maintain and strengthen the European leadership on applications in their respective domains.

MAX has continued to be a leading force in the collaborative efforts that characterise this phase. Its main contribution is in the Applications pillar and the cross-cutting co-design efforts that will be crucial for the overall success of Europe (see activities and deliverables of WP4). MAX has focused on codes and use-cases that will be ready to run on the pre-exascale systems as soon as they will be available (see activities and deliverables of WP1-4 and WP6), and continues to offer training for code developers and users (activities and deliverables of WP8). Overall, the MAX technical work is performed in close synergy with the European stakeholders: this is apparent throughout the technical deliverables of WP1-WP5 and is not the focus of the present D10.6.

Here we concentrate on the activities performed by the MAX leading and management team and all MAX partners to coordinate with the other European stakeholders, in order to elaborate joint strategies and policies and strengthen a synergic and collaborative network and ecosystem. We also report on the strong integration of MAX with the materials research communities in Europe, with active contributions to all the major community organisations and events.

As in the previous reporting period, the effort required by these structuring activities has been larger than initially planned, and often happened on a voluntary basis, thanks to the joint efforts of MAX partners who consider it an investment towards the quality and impact of our future work.

In the following, we first summarise collaborative activities with European organisations in the general HPC ecosystem (Section 2), and then with those belonging to the specific domain of materials research (Section 3). More details on collaborative initiatives of MAX with European institutions on training and education are given in deliverable D8.3.

2. MAX in the European and national HPC ecosystems

MAX has been extremely successful in coordinating and establishing collaborative actions with the key players of the European HPC ecosystem. In this reporting period, we have continued to work with the EC and EuroHPC as described in details below.

2.1 EU and EuroHPC Joint Undertaking

The work and discussions within MAX have been the basis for significant contributions that were offered to the EuroHPC JU and EC in different ways.

- Elisa Molinari has continued to play an active role within the Research & Innovation Advisory Group (RIAG) of the first JU in all its meetings. Its main role is advising on the Strategic research



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and innovation agenda (MSRIA), which identifies priorities for the development and adoption of technologies and key competences for HPC across different application areas. In addition to the general discussion, her specific contributions addressed drafting, discussing and regularly updating:

- the section on “Applications” of the 2020-21 MSRIA (multiannual and periodic);
- the section on “Leadership in HPC use and skills development”, *ibidem*;
- a RIAG recommendation on activities associated with Quantum Technologies (QT) in the EuroHPC Research and Innovation agenda. Elisa Molinari chaired the “QC – HPC working group” that produced the draft recommendations, later unanimously approved by RIAG on August 26, 2021. Members of the working group were: C. Lambert, T. Lippert, J-P Nominé, J-P Panziera, J. VandeVondele, E. Molinari (chair).

MAX was instrumental in preparing data and background work for many of these activities.

- MAX has contributed in different ways to various editions of the EuroHPC **summit weeks**.

Within the **EuroHPC Summit Week 2021**:

- A very successful session was organised: the **MAX workshop on "Computational Materials Design at the Exascale: porting community codes, challenges and success cases"**^{1 2} March 24, 2021, 3 pm. Contributes:
 - Andrea Ferretti (Cnr): Welcome
 - Nicola Marzari (EPFL): Materials design at the intersection of high-throughput and high-performance-computing
 - Stefano Baroni (SISSA): Challenges and success towards the exascale: the perspective of QUANTUM ESPRESSO, a large community code
 - Joost VandeVondele (ETHZ): Software engineering towards exascale: domain specific libraries, communication optimality, and machine learning
 - Daniele Varsano (Cnr): Accelerating GW and many-body perturbation theory using GPUs: Yambo hunting for excitonic insulators
 - Uliana Alekseeva (Jülich): Parallelization and optimization of the FLEUR code: new possibilities for all-electron Density Functional Theory
 - Pablo Ordejón (ICN2): HPC-enabled very large scale quantum simulations in materials with SIESTA
- One more session involving MAX representatives –Elisa Molinari (Cnr & Unimore) and Joost VandeVondele (CSCS ETHZ)– was "Applications Support in EuroHPC - Status and Future: Centres of Excellence in Context". Molinari and VandeVondele were panellists in the "**CoEs on the road to Exascale**"³ Session, organised by FocusCoE, 23/03/2021.

¹ <https://events.prace-ri.eu/event/1018/timetable/#20210324.detailed>

² <http://www.max-centre>

³ <https://events.prace-ri.eu/event/1018/timetable/#20210323.detailed/events/max-coe-workshop-ehpcsw21>



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Within the **EuroHPC Summit Week 2022⁴**, held in Paris on 22-24/03/2022

- MAX has contributed to the organisation of a **Round Table involving all the 15 HPC Centres of Excellence**: "HPC Ecosystem & EuroHPC Day: European HPC CoEs: perspectives for a healthy HPC application eco-system and Exascale" on March 22. There, Elisa Molinari contributed to the first strategic part discussing the need for CoE work across different scales of HPC systems. Andrea Ferretti (CNR) participated in the second technical part talking about complex application workflows in the exascale era.



Figure 1. Tweets about MAX participation at EuroHPC Summit Weeks.

- 23/03/2022. "EUMaster4HPC, the first pan-European Master programme in HPC". Elisa Molinari attended as an invited speaker together with Fabrizio Magugliani (E4).
- 24/03/2022. "User requirements (notably SMEs needs) in HPC". MAX representatives attended the workshop to continue the dialogue with industry stakeholders and users.
- 23/03/2022 several MAX representatives were involved, with invited talks, in the session "HPC for challenging applications: material science": Ivan Carnimeo (SISSA) "QUANTUM ESPRESSO on GPU: accelerating a complex code combining performance with portability"; Daniel Wortmann (Juelich) "Large scale electronic structure simulations of complex magnetic objects"; Marnick Berxc (EPFL) "Generating a FAIR crystal-structure database with the AiiDA informatics infrastructure".
- **Leading the digital decade 1-2/06/2021**

"Leading the Digital Decade" was a two-day online event focused on Europe's digital transformation towards 2030. It was co-organised by the European Commission and the

⁴ <https://events.prace-ri.eu/event/1214/page/142-pracedays22-call-for-contributions>



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Portuguese Presidency of the Council of the European Union.

02/06/2021. Elisa Molinari acted as a panellist in the session about “HPC within the framework of the Digital Europe Programme”.



Figure 2. MAX Tweet and logo of the “Leading the Digital Decade” EU event.

All MAX partners have been especially active within national communities and institutions to promote their commitments towards EuroHPC.

2.2 European CoEs, HPC3, FocusCoE, and National Competence Centres

Together with the other European Centres of Excellence for HPC applications, MAX has worked to build a coordinated ecosystem. We first summarise our contributions to the general coordination activities, and then our specific collaborations with other CoEs.

HPC3, the HPC CoE Council⁵ established in 2019, is formed by the Directors of all the CoEs. It has continued to meet and work in order to ensure that the European HPC CoEs are properly represented in the European HPC ecosystem and in the actions of the EuroHPC Joint Undertaking. The overall goal is to ensure that extreme scale applications result in tangible benefits for addressing scientific, industrial or societal challenges.

MAX has been very active within HPC3, and contributed to identifying and representing common CoEs interests in the European HPC landscape; developing a common point of view on an application-oriented research agenda for HPC in Europe; fostering CoE collaboration and coordination of joint activities. Elisa Molinari served as vice Chairperson of the body, regularly meeting with the Chair, Edouard Audit, and the Secretary, Erwin Laure; they organised meetings with EuroHPC representatives on a few occasions. Luisa Neri and Andrea Ferretti (CNR) served as MAX representatives. The HPC3 met monthly until March 2022, and then quarterly, to share information, define common strategies and organize actions or events with continuous support from the FocusCoE CSA (see below).

⁵ <https://www.hpccoe.eu/hpc-coe-council/>



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FocusCoE⁶, the Horizon2020 Coordination and Support Action (2018-2022), has been working to support the CoEs and HPC3 to more effectively fulfil their role. MAX has actively participated in all its activities, and significantly contributed to the design and coordination of some of them, especially belonging to FocusCoE WP3 (CoE - Industry Interaction), WP5 (Communication, dissemination and outreach), and WP4 (Training). For example MAX, with Francesco Osimanti and Julie Arteza (Trust-IT) and Luisa Neri and Elisabetta Narducci (Cnr), collaborated to WP3, to its survey and to the document “WP3 – Task 3.4 Industrial feedback to CoEs Industry Survey - Summary of results” (from March 2020) and to the *FocusCoE Services Booklet* (see below, from February 2020). Daniele Varsano and M. Celeste Maschio (Cnr) contributed to the Training coordination of WP4. Francesco Osimanti and Rita Giuffrida (Trust-IT) with Luisa Neri (Cnr) contributed to the Promotion initiatives and meeting of WP5.

A detailed list of the MAX contributions to the activities of HPC3 and FocusCoE is given in the Appendix. Besides the active participation in the CSA activities, MAX continuously supported and promoted via its social media the FocusCoE communication activities, and vice versa.

Finally, a major effort was developed in this reporting period towards effective support and **coordination with the National Competence Centres (NCCs)**, recently established at pan-European level (some are still in the early stages of their activity). The initial contacts were coordinated by HPC3, FocusCoE and EuroCC, through presentations at the HPC3 meetings and the preparation of appropriate reference material (e.g., the FocusCoE “*CoEs Service Booklet*”⁷ in April 2022). MAX contributed to two additional *CoE-NCC* meetings (July and September 2022), aimed at defining possible interactions and dedicated actions: Molinari introduced the MAX activities to support the users and developers of applications/platforms, and our offer of hands-on and on-line training. As a first result, an initiative is being organised jointly with ENCCS, the EuroCC National Competence Centre Sweden, is a workshop on “Efficient materials modelling on #HPC with @QuantumESPRESSO, Yambo & BigDFT”⁸ to be held on Nov 14-17, 2022. Further collaborative initiatives with NCCs are under discussion.

2.3 Additional collaborations with individual CoEs

In addition to the common initiatives of all CoEs, some specific MAX collaborations with one or more individual CoEs are presented in the pertinent deliverables. For convenience here we just mention the main collaborations

- **with TRex** (the Centre of Excellence for the community of quantum chemistry):
 - We have continued collaborations on the validation of MAX ground-state results through Quantum Monte Carlo by TRex.
 - We have organised the adoption of our Materials Cloud Archive by TRex, as planned in the TRex proposal. On November 2, 2020 Giovanni Pizzi and Sebastian Huber gave a presentation and a demo of AiiDA+Materials Cloud to the TRex CoE.
 - Both aspects open the way to additional long term synergies.

⁶ <https://www.hpccoe.eu/>

⁷ <https://www.hpccoe.eu/download/>

⁸ <https://enccs.se/events/2022-11-efficient-materials-modelling/>



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- **with Nomad** (another CoE on computational materials science) we are coordinating the universal API OptiMaDe (<http://optimade.org>) for access, exchange and information among all computational databases in Europe and the US. Further joint and coordination initiatives include:
 - The Joint Nomad - E-Cam workshop “Modeling materials at realistic space and time scales via optimal exploitation of exascale computers and AI” (November 2021): N. Marzari (EPFL) held a talk on “Exascale challenges in low dimensional materials”. <https://nomad-coe.eu/events/nomad-e-cam-workshop>;
 - The NVIDIA HPC roundtable on Co-design activity (September 12, 2022) organised to highlight the role of GPU in the materials science codes and identify aspects needed improvement / fixing / implementing: both CoEs attended; for MAX Andrea Ferretti and Nicola Spallanzani (CNR Nano), and Ivan Carnimeo (SISSA);
 - The FAIRmat workshop on data quality in DFT codes co-organized by Nomad (September 2022): Alberto García (CSIC) participated in the roundtable discussion; Gregor Michalíček (Jülich) presented his work on “Challenges in comparing LAPW calculations and estimating their precision”. <https://www.fairdi.eu/events/fairmat-workshop-on-data-quality-in-dft-codes>;
- **with E-CAM** (the CoE on simulation and modelling of materials and biological processes for industry and society) we have worked on:
 - The development of modules in the Electronic Structure Library;
 - A successful collaboration (involving E-Cam, MAX and the Swiss NCCR MARVEL) on the automated generation of Maximally-Localised Wannier Functions to accelerate the design and discovery of materials using first principles high-throughput calculations;
 - Continued collaborations on several training events, and on developing the Lhumos platform (see D 8.3);

Figure 3. MAX tweeted about the collaboration with E-Cam and Marvel.



- **with Nomad, BioExcel, and TRex**, we organised the Workshop on **Co-design for HPC in Computational Materials and Molecular Science** (held in Lausanne October 3-5, 2022): the workshop gathered contributions from leading scientists, technologies, and SW engineers from the fields of academia, HPC centres, HW-vendors, and industry. The workshop covers a broad range of current topics, taking materials and molecular science codes as reference HPC



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applications and possible co-design vehicles: (1) existing examples of HPC co-design in materials and molecular science, (2) co-design of general purpose and domain-specific libraries, kernels, and mini-apps, and (3) the perspective of hardware manufacturers, integrators, and data centre owners. Special focus on (a) the relationship between algorithms and computer architectures in materials science, (b) the connection between parallel programming technologies and runtime systems, and (c) the interplay of the above layers for a wide spectrum of computer architectures, within the selected scientific domain.

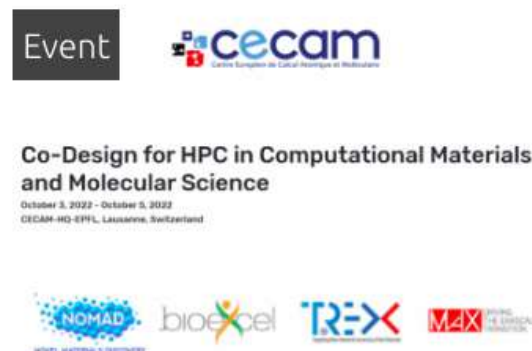


Figure 4. The banner of the news regarding the Co-Design workshop on the MAX website.

For details:

<http://www.max-centre.eu/events/co-design-hpc-computational-materials-and-molecular-science> <https://www.cecama.org/workshop-details/1113>

- **with Excellerat** (the CoE on engineering applications): Excellerat and MAX collaborated on data collection for Market Assessment on the HPC domain, including the analysis of services offered on the EU market. MAX provided some useful information for both the Excellerat Market Assessment (confidential deliverable) and the upcoming Services Portal (public resource). The main sectors covered were: Automotive (batteries, tribochemistry, and tribology), Energy (photovoltaics, batteries, photocatalysis, thermoelectrics), Manufacturing (colorimetry, structural electronic, optical, mechanical properties e.g. for raw materials, metals & minerals, semiconductors for electronics).
- **with EoCoE** (the CoEs on Energy Applications) in December 2020 **we have signed a framework agreement** for collaborations on common interest in the fields of materials research for energy applications, and related scientific and training events. The initial focus was the development of an optimization service of the QUANTUM ESPRESSO-Wannier90 interface. In detail: MAX has optimised and further parallelized the QUANTUM ESPRESSO and Wannier90 routines responsible for generating Wannier functions; while EoCoE provided realistic and computationally demanding test cases of increasing cell size to test the scaling and validate the new optimised kernels. EoCoE also acted as beta tester of the software improvements, providing feedback about the numerical and parallel performance of Quantum ESPRESSO and Wannier90 when used on EoCoE scientific cases of interest.
- **with EoCoE and Hidalgo** (the CoE on Global systems) we have collaborated on the 2021 edition of EUSEW, the European Sustainable Energy Week (25-29/10/2021), dedicated to Towards

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2030: Reshaping the European Energy System: we have organised a dedicated session on “HPC and Big Data as key enablers” (see figure 5).

- **with Pop** (the CoE on Performance Optimisation and Productivity in HPC): In the final period of the project we made agreements for a new profiling campaign on MAX codes by Pop staff. We have collected from the MAX developers the information requested by Pop regarding some structural features of the codes, such as the parallelization techniques implemented, the libraries used, case studies on which to perform the profiling, etc., and look forward to the next steps by Pop.



Figure 5. MAX tweet about EUSEW2021.

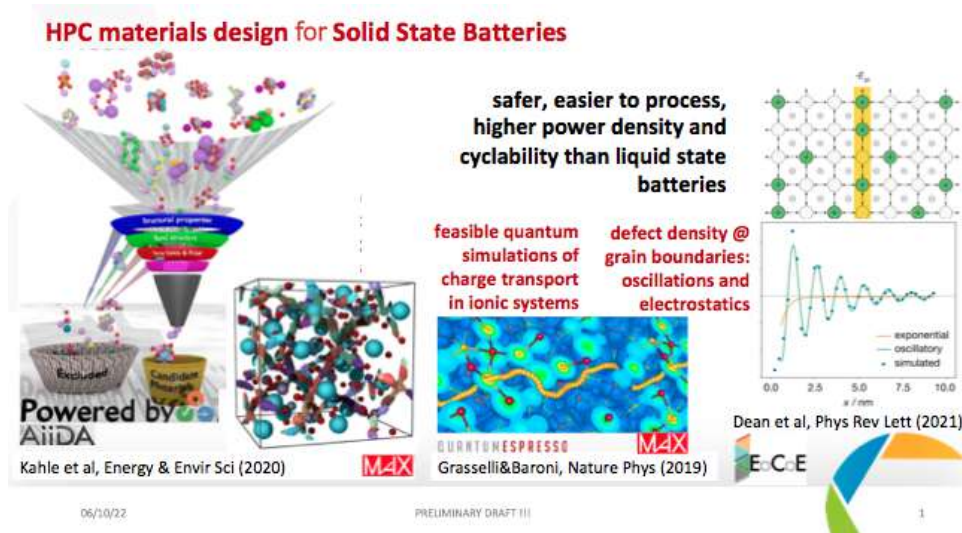


Figure 6. A slide from the MAX contribution to Eusew 2021. The focus was on HPC as a key tool for the predictive design of materials for energy, and accelerated innovation in energy technologies. Here challenges and results in materials for solid state batteries are shown as an example. On the left the MAX high throughput workflow for the predictive design of solid state electrolytes, based on Aiida and QUANTUM ESPRESSO, and a new approach to simulate charge transport from first principles. On the right a complementary contribution from EoCoE on defects at grain boundaries.



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2.4 EOOSC, ETP4HPC, EPI and technology projects

MAX partners took part in the activities of **EOOSC and EOOSC-Hub, and ETP4HPC** as described below.

1. EOOSC

MAX, EOOSC and EOOSC-Hub have continued their collaboration, along the lines that were set up in the previous reporting period. The overall purpose is to offer and maintain a platform for reproducible science with full provenance along the lines defined in MAX WP5, based on AiiDA, AiiDALab, and the Materials Cloud Archive, all co-developed by MAX.

The [Materials Cloud Archive](https://marketplace.eosc-portal.eu/services/materials-cloud-archive) is maintained and available as a long-term FAIR data repository for computational materials science <https://marketplace.eosc-portal.eu/services/materials-cloud-archive>. The site guarantees access to the repository with long-term storage (for at least 10 years) of data records and associated metadata, their findability via persistent identifiers (including a DOI), and their accessibility via standard protocols. Submissions are moderated to ensure their completeness, adherence to the FAIR principles, and relevance to the field of materials science. This service is supported by a large number of partners including MAX.

The screenshot shows the 'Materials Cloud Archive' service page on the EOOSC Marketplace. At the top, there is the 'EUROPEAN OPEN SCIENCE CLOUD' logo and a search bar. Below the logo, the breadcrumb trail reads: 'Resources > Sharing & Discovery > Data > Scientific/Research Data > Materials Cloud Archive'. The main content area features the 'Materials Cloud Archive' logo, a description: 'A long-term FAIR data repository for computational materials science', and the organization 'Materials Cloud'. There are also star ratings (0.0/5) and buttons for 'Add to comparison' and 'Add to favourites'. A prominent blue button says 'Access the resource'. Below this, there are links for 'Webpage', 'Helpdesk e-mail', and 'Manual'. A section titled 'SCIENTIFIC CATEGORISATION' shows icons for 'Natural Sciences' and 'Engineering & Technology'. At the bottom, a paragraph describes the archive as an open-access, moderated repository for research data in computational materials science, guaranteeing long-term storage (at least 10 years) and FAIR principles.

Figure 7. Materials Cloud Archive service page on the EOOSC hub Marketplace catalogue.

AiiDA, the workflow manager with a strong focus on provenance and performance, is maintained and made available at <https://marketplace.eosc-portal.eu/services/aiida-lab>. Through its flexible plugin infrastructure, AiiDA supports a wide range of simulation codes including the MAX flagship codes, and automatically records the full provenance of a simulation pipeline in a graph. **AiiDALab** allows the user to run and manage AiiDA-powered workflows through tailored web applications in the browser. The apps can be picked and installed from the application registry in the App store, or written by the users



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in a few lines of python using jupyter widgets and appmode. This service is supported by MAX, MARVEL NCCR, the European H2020 MarketPlace project, and a number of other partners.

The screenshot shows the AiiDALab service page on the EOSC Marketplace. At the top, there's a search bar and 'My EOSC Marketplace' link. The main header includes the EOSC logo and 'EUROPEAN OPEN SCIENCE CLOUD'. Below that, a breadcrumb trail reads: 'Resources > Access physical & infrastructures > Compute > Other > AiiDALab'. The service card for AiiDALab features the logo, a description: 'Reproducible turn-key workflows for materials science', and 'Organisation: Materials Cloud'. It has a rating of 0.0/5 with 0 reviews and buttons for 'Add to comparison' and 'Add to favourites'. A prominent blue button says 'Access the resource' with 'OPEN ACCESS' below it. Navigation links include 'Webpage', 'Helpdesk e-mail', 'Manual', and 'Training information', along with a link to 'Ask a question about this resource?'. The page has tabs for 'ABOUT', 'DETAILS', and 'REVIEWS (0)'. Below the service card, there's a paragraph describing AiiDA as a workflow manager for computational science, focusing on provenance and performance. To the right, a 'SCIENTIFIC CATEGORISATION' section shows 'Natural Sciences' and 'Chemical Sciences' with expandable arrows.

Figure 8. AiiDALab service page on the EOSC hub Marketplace catalogue.

The screenshot shows the MAX page in the European Science Cloud Catalogue. At the top, it says 'MAX Materials design at the eXascale'. Below the MAX logo, there's a list of project details: 'PROJECT WEBSITE: https://www.max-centre.eu', 'CONTACT E-MAIL: info@max-centre.eu', 'START DATE: 2022-01-01', 'END DATE: 2025-12-31', 'FUNDS PROGRAMME: Horizon Europe', 'FIELD OF EXPERTISE: High-Performance Computing, Materials Science, and Data Science', and 'DOI: 10.54455/2022-01-01'. The 'TARGET USERS' section lists 'Academy/Research Institutes', 'Research Centres', 'Government/Policy Administration', 'Users in Industry', 'Small & Medium Enterprises', 'Data Centres', 'Data Providers', and 'Through existing partners'. The 'ENGAGEMENT WITH EOSC' section includes a paragraph about contributing to EOSC and a list of 'POTENTIAL AREAS OF COLLABORATION WITH THE EOSC' such as 'EOSC Core Horizontal Services', 'Federated Data', 'EOSC Exchange', 'Services for the Long Tail of Science', 'FAIR Services & Practices', and 'Future Governance of EOSC'. The 'COMMUNITY ENGAGEMENT' section features 'TRAINING' and 'USES CASES'.

Figure 9. MAX page in the European Science Cloud Catalogue.

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2. ETP4HPC

ETP4HPC, the European Technology Platform for HPC, is an industry-led think-tank aiming to promote HPC research and innovation. Its main contribution consists in strategic documents on technology developments, often referred to in broader EC and EuroHPC work programs. Several MAX researchers have continued to participate in these efforts, based on lessons learned in MAX. MAX partners who are leading members of the ETP4HPC (among them C. Cavazzoni, F. Magugliani) have been active in shaping SRA5, the **fifth edition of the Strategic Research Agenda**, published in October 2022 (<https://www.etp4hpc.eu/sra.html>), especially the parts on Applications and on Training and Education.

Moreover, MAX has collaborated on the 2020 and 2021 editions of the **Etp4HPC Handbook of EU HPC projects** (2020 and 2021 editions, released on 6/11/2020 and 9/09/2021), available for download at <https://www.etp4hpc.eu/european-hpc-handbook.html>



Figure 10. The covers of the Etp4HPC Handbook of EU HPC i) edition 2020; ii) edition 2021, and the cover of the fifth edition of the Strategic Research Agenda 2022.

2.5 Technology collaborations

The overall collaborations on technology are summarised in D4.6. MAX has continued to systematically collaborate with **EPI –the European Processor Initiative–** and started interacting with other technology projects, in particular EUPEX in collaboration with CINECA. With EPI we share co-design initiatives, and have been communicating findings about MAX codes and co-design vehicles (mini-apps, libraries). In particular, EPI has adopted the LAXlib miniapp from QUANTUM ESPRESSO, the DBCSR library from CP2K, as well as the BigDFT application. Together with ARM, in MAX we have continued work to validate the codes and mini-apps on ARM architecture and deliver performance evaluations on simulated and



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emulated SVE instruction sets. Some of the MAX flagship codes have been evaluated on AWS Graviton3, relevant e.g. for the SiPearl RHEA chip (tightly connected to the outcome of the first phase of EPI) and NVIDIA Grace. Profiling information was shared with EPI, to assure the vectorization level available in the future EPI processor as well as the size of the different cache levels will be adequate for MAX applications. Preliminary tests that we have done on real ARM processors with SVE (made available to MAX through Cineca by Fujitsu) show encouraging performances and no major bottlenecks with respect to the memory, cache, and vectorizations.

In this scenario, direct interactions with Atos and SiPearl have started, especially focused on co-design actions. We also acknowledge tight and continuous collaboration (e.g. in the form of common initiatives and software development) with NVIDIA, INTEL, and AMD personnel for what concerns the support and exploitation of the different software stacks for GPU acceleration.

2.6 PRACE and pre-exascale HPC Consortia, EUMaster4HPC

MAX is committed to making codes running and performing on HPC machines in Europe (and beyond). For this reason, it has been collaborating systematically with **PRACE** –the Partnership for Advanced Computing in Europe– that has been providing competitive access to the Tier 0 European supercomputers in the last years. The main collaborative activities performed by MAX include:

- MAX high level domain specific support to users of MAX codes to prepare computational projects for PRACE calls: this resulted in a large number of successful PRACE projects (see figure 11);
- collaboration with work packages dealing with codes, benchmarks and libraries: some of the MAX codes are included in the PRACE benchmark suite.⁹
- coordination of MAX high level domain specific training with training actions offered by PRACE, and specific contributions from MAX in joint events with PRACE

⁹ <https://prace-ri.eu/training-support/technical-documentation/benchmark-suites/>



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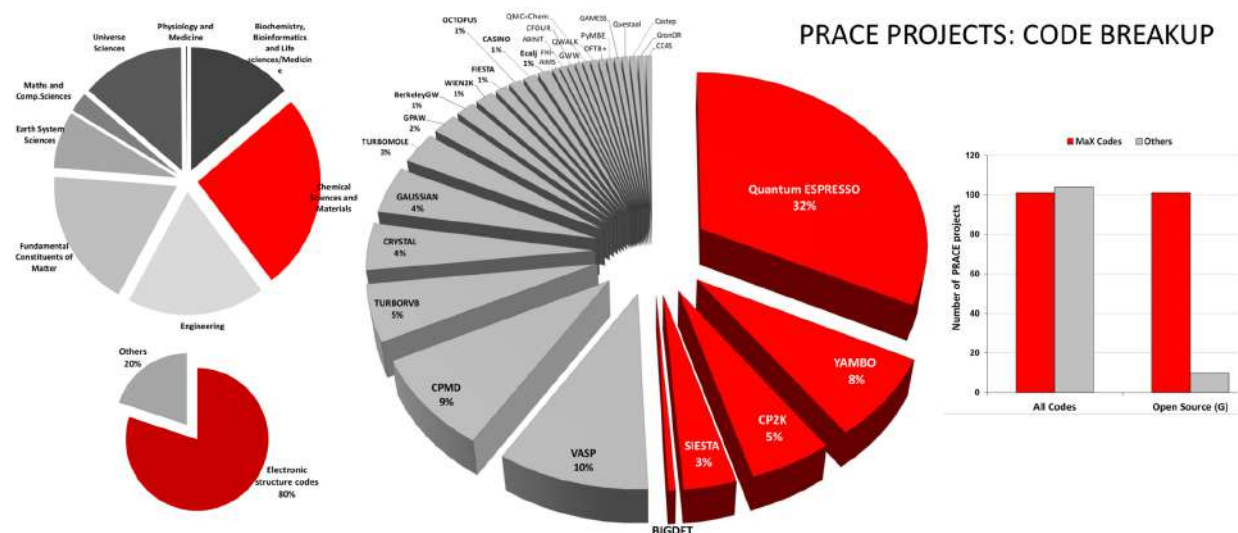


Figure 11. Number of PRACE granted projects using a given code, within the ‘Chemistry and Materials Science’ domain. Only ‘electronic structure-based’ codes are considered in this slide. The central pie shows that in the materials domain European codes are leading, and MaX flagship codes (in red) play a key role. The histograms on the right show that MaX codes represent over 80% of the open-source component. Source: MaX elaboration from Prace data (calls from 1 to 23), 2021.

In addition, MAX has extensively collaborated with PRACE in several of their training courses.

Since the initial decisions on the new EuroHPC supercomputers –especially the pre-exascale machines–, that will be run by new Consortia, MAX has started close interactions in order to prepare for the best use and performance of codes, in particular on the heterogeneous architectures. We have promoted **joint meetings of HPC3 with the LUMI and the Leonardo consortia**, and plan to do the same with **BSC** as soon as possible, now that the procurement of that machine is closed. After a number of direct e-mail exchanges concerning MaX needs and collaboration opportunities, we have also run **dedicated MAX-LUMI and MAX-Leonardo on-line meetings**, and their representatives participated in **MAX developers events** together with AMD and NVIDIA experts. More details about the results of MAX code porting to the new machines are the subject of WP4 deliverables and future work, and we are confident that the collaborative efforts will continue to be effective in the next stages of the infrastructure deployment.

As far as formal agreements with new and future HPC facilities, recent meetings with EuroHPC (Daniel Opalka) and the coordinator of the new Castiel CSA (Bastian Koller) indicated that CoEs will take advantage of support/coordination by Castiel: this seems reasonable given the many common issues. Work is ongoing in that direction, and meanwhile we are working on specific additional agreements that MAX will need.



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A new significant collaboration has started in the last year with the **EUMaster4HPC** –the HPC European Consortium Leading Education Activities–, a new European initiative that is developing a new European Master programme focusing on HPC advancements and applications into different scientific and industrial domains. MaX representatives have contributed in particular to designing a project Task aimed at synergies and coordination between this new curriculum and existing Master courses in different disciplines, including, e.g., Physics, Chemistry, Materials Sciences and Engineering. MaX is promoting “Materials” as one of the pilot domains for the exchange of innovative domain-specific education tools, materials and experiences.

EUMaster4HPC emphasises collaboration across Europe with innovative teaching paradigms including co-teaching and the cooperative development of new content relying on the best specialists in HPC education in Europe. Employers, researchers, HPC specialists, supercomputing centres, CoEs and technology providers will constitute a workforce towards this master in HPC pilot programme. This pilot will provide a base for further national and pan-European educational programmes in HPC all over Europe and our lessons learned and the material development will accelerate the uptake of HPC in academia and industry.

The creation of a European network of HPC specialists will catalyse transfers and mutual support between students, teachers and industrial experts. A particular focus on mobility of students and teachers will enable students to rapidly gain experience through internships and exposure to European supercomputing centres.

3. MAX in the HPC materials research ecosystem in Europe and beyond

Within this deliverable we report on MAX activities to strengthen collaborations with communities in Europe, that can best take advantage of materials science codes and of the future EuroHPC supercomputers, and with communities worldwide which are/can be users/developers of MAX codes thereby enhancing their impact.

Psi-k network

[Psi-k](#) is a Europe-based, worldwide network of researchers working on the advancement of first-principles computational materials science, supported bottom-up by research groups in the scientific community. Key activities of Psi-k are the organisation of conferences, workshops, tutorials and training schools (typically ~30 every year, and a general conference with 1000+ participants every 5 years) as well as the dissemination of scientific thinking in society. Psi-k produces a regular [newsletter](#) with extensive scientific highlights, and allows researchers to advertise job openings, events, etc through its 5000+ members [mailing list](#).

MAX partners are among the leading participants of the Psi-k network (N. Marzari has been the chair, E. Molinari and S. Blugel are Trustees, several MAX partners are members of the Scientific boards and working groups). MAX has established structured collaborations through several coordination meetings,



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aimed at disseminating MAX results in the scientific community and engaging prospective users. This resulted in:

- Co-organization and support of several specialised workshops (reported in D8.3):
 - All-electron DFT with Fleur - A Hands-on Tutorial - online from April 12 to, 2021, *MAX Organisers and speakers: Daniel Wortmann, Uliana Alekseeva, Gregor Michalick, Stefan Blügel, Jens Bröder, Matthias Redies (Juelich), and Francisco Fernando Ramirez (EPFL).*
 - Young Researcher's Workshop on Machine Learning for Materials - SISSA Miramare Campus Trieste (IT) from May 9 to 13, 2022, *MAX Organisers and speakers: Stefano de Gironcoli (SISSA), Alessandro Laio (SISSA).*
 - Wannier 2022 Summer School ICTP - Trieste (Italy) and online from May 16 to 20, 2022, *MAX Organisers and speakers: Giovanni PIZZI (EPFL), N. Marzari (EPFL, Switzerland).*
 - ESL Workshop 2021: Extended Software Development Workshop: Improving bundle libraries- CECAM-HQ-EPFL, Lausanne, Switzerland from October 11 to October 22, 2021, *MAX Organisers and speakers: Emilio Artacho (ICN2), Giovanni Pizzi (EPFL), Michele Ceriotti (EPFL), Alberto Garcia (CSIC), Stefano de Gironcoli (SISSA), Anton Kozhevnikov (ETHZ).*
 - Optimising Digital Teaching and Communication - online from September 15 to October 1, 2021, *MAX Organisers and speakers: Stefaan Cottenier (Ghent University).*
- Dissemination of *MAX* openings and events through the Psi-k mailing list.
- Participation of MAX to the Psi-k Conference 2022 in Lausanne (August 22-25, 2022) with dedicated activities:
 - **MAX booth** (throughout the entire duration of the conference) with the aim to disseminate MAX work and latest codes' advancements, to offer the opportunity to meet the MAX code developers. For this purpose we prepared 10 dedicated factsheets: a general one to present MAX facts and figures and 9 for the flagship codes (printed as giveaways during the conference and digital, available for download on MAX website).
 - **MAX Happy Hour** a dedicated event on Tuesday evening, Aug 23 after the end of the Conference session, with a short overview on MAX results, a buffet dinner, and a users meeting with the developers of MAX codes.
 - **MAX talks and posters:** MAX partners performed several talks, posters and chaired several symposia during the whole conference.

CECAM

CECAM (Centre Européen de Calcul Atomique et Moléculaire) promotes fundamental research on advanced computational methods and their application to important problems in frontier areas of science and technology. 24 Institutions from 14 European countries, including Ministries, National



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Research Councils, Research and High Performance Computing Centres, Universities, fund CECAM and concur in defining its strategy and activities.

Several MAX partners are among leading members in CECAM boards, and MAX participates in structuring strategy and policy discussions together with CECAM. An important example is

- the **“Scout” meeting** to consolidate common activities or explore novel collaborations between CECAM and projects, partnerships, and relevant players in the areas of software development in the evolving landscape of high performance computing, and data driven discovery (computational and experimental). This meeting was finally held on October 24-25, 2022, but prepared through several previous discussions within the present reporting period. Speakers from MAX included Joost VandeVondele (CSCS) and Fabio Affinito (Cineca) on HPC Centres and scientific communities, Elisa Molinari on synergies between Cecam and CoEs and HPC3, Nicola Marzari on strategic opportunities for collaboration between CECAM and the Swiss NCCR, Thierry Deutsch on initiatives on data drive science and large scale infrastructures. Andrea Ferretti (CNR-NANO) also attended as MAX representative.

Importantly, MAX has established a structured collaboration with CECAM, especially aimed at collaborative training events. Within this reporting period, these included especially co-organization and support of several schools (see also D8.3):

- Virtual school on electronic excitations in solids and nanostructures using the Yambo code - online on April 8-9 and 15-16, 2021, *MAX organisers and speakers*: Daniele Varsano (CNR), Fulvio Paleari (CNR ISM), Dario A. Leon Valido (CNR Nano), Andrea Ferretti (CNR Nano), Samaneh Ataei (CNR Nano), Alberto Guandalini (CNR Nano), Davide Sangalli (CNR ISM), Andrea Marini (CNR ISM), Nicola Spallanzani (CNR Nano), Pedro Melo (CNR ISM), Miki Bonacci (CNR Nano), Matteo Zanfrognini (CNR Nano), Pino D'Amico (CNR Nano), Claudia Cardoso (CNR Nano), Ivan Marri (CNR Nano and Unimore), Ridwan Agbaoye (CNR Nano).
- All-electron DFT with Fleur - A Hands-on Tutorial - online from April 12 to, 2021, *MAX organisers and speakers*: Daniel Wortmann, Uliana Alekseeva, Gregor Michalicek, Stefan Blügel, Jens Bröder, Matthias Redies (Juelich), and Francisco Fernando Ramirez (EPFL).
- Advanced school on Quantum Transport using SIESTA - online from May 17 to 21, 2021, *MAX organisers and speakers*: Pablo Ordejon (ICN2).
- First-principles simulations of materials with SIESTA - online from June 28 to July 2, 2021, *MAX organisers and speakers*: José María Escartín Esteban (ICN2), Alberto Garcia (ICMAB-CSIC), Pablo Ordejon (ICN2), Miguel Pruneda (ICN2), Arsalan Akhtar (ICN2), Ernane De Freitas Martins (ICN2), Vladimir Dikan (ICMAB-CSIC), Roberta Farris (ICN2), Alberto Garcia (ICMAB-CSIC), Xu He (ICN2), Federico Nicolás Pedron (ICN2), Miguel Pruneda (ICN2), Nils Wittemeier (ICN2), Emilio Artacho (University of Cambridge and ICN2).
- Ab-initio Many-Body Methods and Simulations with the Yambo Code - hybrid, online and at ICTP Kastler Lecture Hall from April, 4 to 8, 2022, *MAX organisers and speakers*: Andrea Marini



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(CNR-ISM), Davide Sangalli (CNR-ISM), Daniele Varsano (CNR-NANO), Alberto Guandalini (CNR-NANO), Dario Alejandro Leon Valido (CNR-NANO), Fulvio Paleari (CNR-NANO).

- Young Researcher's Workshop on Machine Learning for Materials - SISSA Miramare Campus Trieste (IT) from May 9 to 13, 2022, *MAX Organisers and speakers*: Stefano de Gironcoli (SISSA), Alessandro Laio (SISSA).
- Wannier 2022 Summer School ICTP - Trieste (Italy) and online from May 16 to 20, 2022, *MAX Organisers and speakers*: Giovanni PIZZI (EPFL), N. Marzari (EPFL, Switzerland).
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- Optimising Digital Teaching and Communication - online from September 15 to October 1, 2021, *MAX Organisers and speakers*: Stefaan Cottenier (Ghent University).

Last but not least, MAX is collaborating with CECAM and MARVEL on the development of Lhumos, a web portal for educational material for modelling and simulations of materials, presenting a user-friendly environment for uploading and viewing data (video-lectures, training materials), including metadata control protocols and effective management of tags for content (see D8.3). The deployment, expected in early 2023, will be directly integrated in the MaX website; further integration steps with broader European portals will also be pursued as they become available.

OPTIMADE

MAX (with Materials Cloud) and over 30 other research institutions have come together to form the Open Databases Integration for Materials Design consortium and develop an API specification enabling seamless access and interoperability among materials databases. This work has been included in the open access paper "[OPTIMADE, an API for exchanging materials data](#)" published on 12/08/2021 in Scientific Data, a Nature Research's journal. For additional details we refer to this paper, which presents the OPTIMADE API specification, illustrates its use and discusses future prospects and ongoing development, and to deliverable D5.5.

GO-FAIR

MAX has continued to participate in the official Go-FAIR implementation networks (INs) (<https://www.go-fair.org/implementation-networks>) through the Materials Cloud consortium. As such, it is committed to defining and creating specific materials and tools as elements of the Internet of FAIR Data and Services (IFDS), to foster a community of harmonised FAIR practices, and to communicate on critical issues on which consensus has been reached and which are of importance for the community.



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EMMC

EMMC, the European Materials Modelling Council, is an organisation promoting materials modelling with focus on industrial research and innovation. MAX has contributed to the 2020 The EMMC Roadmap for Materials Modelling and Digitalisation of the Materials Sciences.¹⁰ MAX representatives attended the [3rd EMMC International Workshop 2021](#), 2-4/03/2021 with the following contributions:

- Plenary session - Day 2 - 03/03/2021 - invited talk by Nicola Marzari (EPFL) “The digital infrastructures for 21st-century science”,¹¹
- Open Contributions and Virtual Stands Session of Andrea Ferretti and Daniele Varsano titled “A journey through electronic structure and materials modelling at the exascale”.¹²

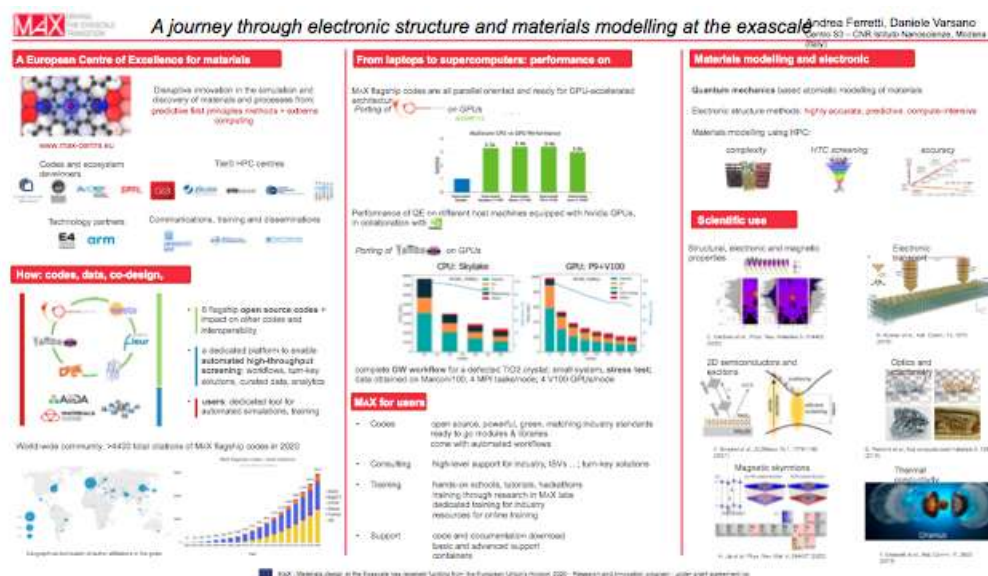


Figure 12: Poster presented @ the 3rd EMMC International Workshop 2021.

- contribution to the Policy Session10 which gave a high-level overview of the [Roadmap](#), and defined directions on gaps and challenges for the next version of the Roadmap with feedback from MAX partners.

ETSF

ETSF, the European Theoretical Spectroscopy Facility, is a knowledge centre for theoretical spectroscopy and a network of researchers carrying out state-of-the-art research on theoretical and computational methods for studying electronic and optical properties of materials. Several MAX members participate,

¹⁰ <https://zenodo.org/record/4272033#.Yz6ulexBwUR>

¹¹ <https://emmc.eu/wp-content/uploads/2020/12/EMMC2021-P4-Marzari-Abstract.pdf>

¹² <https://drive.google.com/drive/u/0/folders/1jqPp4SC3EPBPPfdtimMwJvKqUnlambE>



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D. Varsano (CNR) is a member of the steering committee, and the MAX flagship code Yambo is a reference code for the ETSF community. MAX has worked to ensure the best use of MAX codes and ETSF members were involved as lecturers in the event Ab-initio Many-Body Methods and Simulations with the Yambo Code (April 2022). ETSF is particularly interested in training and e-learning events. In this regard, MAX and ETSF have conceived and implemented the event: Optimizing Digital Teaching and Communication (September-October 2021).

Batteries and BIG-MAP initiatives

Research on future batteries is a huge field for computational materials simulation and design, coordinated in the Battery2030+ initiatives, including BIG-MAP,¹³ the large project on "Battery Interface Genome - Materials Acceleration Platform" with its large industrial component. The BIG-MAP vision is to develop a modular, closed-loop infrastructure and methodology to bridge physical insights and data-driven approaches to accelerate the discovery of sustainable battery chemistries and technologies. BIG-MAP's strategy is to cohesively integrate machine learning, computer simulations and AI-orchestrated experiments and synthesis to accelerate battery materials discovery and optimization. MAX participates in these initiatives through the CNR, EPFL and ICN2-CSIC teams.

In addition to supporting specific research tasks on computational spectroscopies and data management, MAX has worked to ensure the best use of MAX codes and data platforms, and of the whole EuroHPC ecosystem, within that community. We have actively participated in many discussions, including the Second Biannual Meeting on Big-Map project - Copenhagen (DK) - 16-17/09/2021 (Elisa Molinari and Deborah Prezzi) and other bilateral and informal exchanges.

National initiatives in Europe

Concerning national initiatives in Europe, MAX is well connected and active in most countries through its partners. Here we mention only a few selected cases where the CoE is involved in collaborations with significant impact:

MARVEL, Switzerland

MARVEL is a Swiss centre on computational design and discovery of novel materials, created in 2014 and recently renewed until 2026. Together with MAX, MARVEL contributed to the development and the long term sustainability of the Materials Cloud (<https://www.materialscloud.org/>), a platform built to enable the seamless sharing and dissemination of resources in computational materials science. Through the Materials Cloud MAX offers educational, research, and archiving tools; simulation software and services; and curated and raw data that underpin published results and empower data-based discovery, compliant with data management plans and the FAIR principles.

Italian National Research Centre in High Performance Computing, Big Data e Quantum Computing

Within the NextGenerationEU plan, a number of HPC-related initiatives have recently started in Italy. The most important one is the new "National Research Centre in High Performance Computing, Big

¹³ <https://www.big-map.eu>



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Data e Quantum Computing”, funded with 320MEuro, that will be co-located in a new site together with the Leonardo supercomputer in Bologna. Beside facilities, the initiative comprises vertical thematic pillars, and one of them is “Materials”. It is fair to say that MAX and its partners have taken the lead in shaping this pillar, which includes the main Italian teams and will enable a few tens of post-docs and PhD students in our domain. Through similar funding lines, a few related initiatives are starting at regional level: MAX partners are looking forward to enabling and supporting them too.

Associazione BIGDATA (ABD), Italy

ABD is an association involving the main actors in Italy in the HPC and big data domains (<https://associazionebigdata.it/>). Among the activities promoted by ABD is the large project “SUPER - Supercomputing Unified Platform - Emilia-Romagna”, supported by the Emilia-Romagna region POR-FESR program, which was recently completed (February 2022). SUPER has supported the uptake of MAX codes and their application to a few use cases of industrial relevance.

Other European countries

In addition, we have especially focused on **countries which are not yet fully integrated/supported in the European HPC system**, such as EU13 countries. A few examples of activities to broaden the MAX impact in new countries included:

- presentations by Nicola Marzari (EPFL) in the first Austrian-Slovenian HPC Meeting ASHPC21 (Keynote talk on 13/05/2021, online) and in a Webinar at the Cyprus Institute (23/11/2021) on “The great acceleration in the design and discovery of novel materials” (<https://ashpc21.si/>; <https://www.cyi.ac.cy/index.php/component/k2/webinar-the-great-acceleration-in-the-design-and-discovery-of-novel-materials.html>);
- keynote talk by Pablo Ordejón (ICN2) at the TNT2021 Conference in Tirana (Albania, 06/10/2021) titled “Towards first-principles electrochemistry: Addressing electrified metal-electrolyte interfaces with DFT-NEGF” (<https://tntconf.org/2021/programme.php?d=06>).

Of special relevance are the discussions that were initiated to develop collaborations with two centres in the Czech Republic and in Slovenia: the IT4Innovations National Supercomputing Centre - Technical University Ostrava (CZ) and the Jozef Stefan Institute (SI). The actual collaborations have just started, but the discussions finally led to their participation in the partnership of the next MAX proposal.

Non EU-country initiatives

Concerning non EU-country initiatives, MAX continuously interacted with similar Centres on Materials design worldwide.

Close interactions have meanwhile been strengthened with the **computational materials centres in the US**: Marzari (EPFL) is the Chair of the Scientific Advisory Board of MICCoM, the DOE Midwest Integrated Center for Computational Materials at the University of Chicago and Argonne National Laboratory, together with Steven Louie (UC Berkeley), himself the director of the DOE Center for Computational



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Study of Excited-State Phenomena in Energy Materials. These close interactions provide optimal synergies between the US activities and the MAX efforts.

MAX has maintained close interactions with the **materials science community in Africa**, thanks to the activities of ASESMA (the African School on Electronic Structure Simulations and Applications), where Marzari (EPFL) has been active since its creation in 2010, and is part of the International Advisory Board.

Japan. Materials sciences are a key component of HPC-based research on frontier supercomputers in Japan. The EU is therefore exploring possible collaborations. An "EU-Japan workshop on HPC-based material sciences" was jointly promoted by the EC and RIKEN on November 9 and 10, 2022, to discuss the possibility of common initiatives on HPC-based materials simulation and informatics (with a view to collaboration in Horizon Europe in the near future). MaX representatives contributed to the organization (Elisa Molinari co-chaired the workshop on the EU side, together with Edouard Audit), and Thierry Deutch (CEA) gave one of the presentations. A discussion on possible challenges for collaboration started, especially on applications/codes and how they will be impacted by pre- and exascale architectures (e.g. re-design, recoding for accelerators). Satoshi Matsuoka, Director of the Center for Computational Science at RIKEN, also proposed to focus on how such applications in primary target areas such materials may influence the design and architectures of the future systems. The discussion on prospective joint support actions and calls is ongoing, with the coordination by L. Flores on the EC side.

Interactions with international institutions and organizations have passed through the wide activity of scientific and institutional dissemination. All speakers have always cited the MaX contribution to their work and its relevance and opportunities for related activities. A complete list of talks is given in D9.4, Annex III).

4. Conclusions

MAX is now recognized as a cornerstone of the European application and HPC ecosystem, and as a reference point for the computational materials research community in Europe and beyond. Its main contributions come undoubtedly from the work of the technical work packages, performed in close synergy with the European HPC stakeholders and with the materials research community, as apparent in all the technical deliverables of WP1-WP8.

Here we have highlighted how such contributions have been constantly accompanied by an effort to elaborate joint European strategies and policies, and to strengthen a synergic and collaborative network and ecosystem in Europe. The MAX leading and management team and all MAX partners have coordinated with the other European stakeholders and contributed to all the major EU community organisations and events.

In the last period, with the actual start of the EuroHPC petascale and especially pre-exascale machines, as well as the decisions on forthcoming architectures, we are establishing/consolidating collaborations with the relevant Consortia and actors. At the same time, we strengthened the main collaborative



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activities reported in the previous deliverable D10.3. For example, we have documented much stronger collaborations with CoEs, their ecosystem and EuroHPC projects as a whole, and the main European community networks in the materials domain.

We are confident that the large effort required by the structuring activities described in this deliverable may constitute a fruitful investment towards the quality and impact of our future work.



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APPENDIX

MAX ACTIVE PARTICIPATION IN JOINT FocusCoE and HPC3 INITIATIVES

Meetings organized by FocusCoE

1. 14/10/2020. *FocusCoE-CoEs workshop*: a workshop to ensure broader information and feedback on FocusCoE activities, and plan further collaboration of HPC3 and FocusCoE.
 2. 20/11/2020. *EuroHPC-CoE Briefing by Juan Pelegrin* (about the status of planning for CoEs in the context of EuroHPC).
 3. 1/3/2022. *Intel OneAPI Workshop brought to you by FocusCoE¹⁴*. Presentations by Intel experts covering the OneAPI vision, design, toolkits, a use case with GROMACS, and specific tools for migration and debugging.
- **FocusCoE & CoEs WP3.**
 4. 16/06/2020; 24/06/2020; 30/09/2020 Joint telcos of FocusCoE WP3 and CoE representatives.
 5. *Meetings on interaction with industries*: ; 03/02/2021; 18/05/2021; 7/09/2021; 16/09/2021.
 6. 05/11/2020. *FocusCoE sustainability workshop, Day 1* (with a presentation about *Sustainability @ MAX* by Luisa Neri)
 7. 27/11/2020 & 04/12/2020. *Business Webinar: Interaction with Industry and SME*.
 8. 21/01/2021. *FocusCoE sustainability workshop, Day 2*.
 - **FocusCoE & CoEs Training WP4.**
 9. 02, 03, 09/11/2020. CodeRefinery instructor training workshop for HPC CoEs in collaboration with FocusCoE and HPC Carpentry.
 10. 20/10/2021. Training Portal updates.
 11. 07/03/2022. definition of the portal for European HPC services.
 12. 26/03/2021 MAX contributed to the *FocusCoE training session* at EHPCSW21: HPC education and training – perspectives from EU13 Member States. The workshop focused on the HPC education and training landscape among the EU13 Member States, mainly on existing programmes, target communities and industries, and future perspectives.
 13. 09/04/2021 FocusCoE “Sustainability Training Workshop - Morning session” (M.C. Maschio - CNR).
 - **HPC3 meetings**
 14. 10/06/2020. HPC CoE Council Meeting #11 (telco).
 15. 08/07/2020. HPC CoE Council Meeting #12 (telco).
 16. 09/09/2020. HPC CoE Council Meeting #13 (telco).

¹⁴ <https://www.hpccoe.eu/2022/03/04/focuscoe-hosts-intel-and-eu-hpc-coes-for-oneapi-workshop/>



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17. 11/11/2020. HPC CoE Council Meeting #14 (telco).
 18. 16/12/2020. HPC CoE Council Meeting #15 (telco).
 19. 20/01/2021. HPC CoE Council Meeting #16 (telco).
 20. 17/02/2021. HPC CoE Council Meeting #17 (telco).
 21. 18/03/2021. HPC CoE Council Meeting #18 (telco).
 22. 14/04/2021. *Fitness Check preparatory meeting* (22/04/2022). Preparation of a common CoEs' document "CoE's achievements, problems and perspectives" for the EU fitness check.
 23. 21/04/2021. HPC CoE Council Meeting #19 (telco).
 24. 19/05/2021. HPC CoE Council Meeting #20 (telco).
 25. 16/06/2021. HPC CoE Council Meeting #21 (telco).
 26. 18/08/2021. HPC CoE Council Meeting #22 (telco).
 27. 13/09/2021. HPC CoE Council Meeting #23 (telco).
 28. 20/10/2021. HPC CoE Council Meeting #24 (telco).
 29. 17/11/2021. HPC CoE Council Meeting #25 (telco).
 30. 15/12/2021. HPC CoE Council Meeting #26 (telco).
 31. 19/01/2022. HPC CoE Council Meeting #27 (telco).
 32. 16/02/2022. HPC CoE Council Meeting #28 (telco).
- **Meetings CoE and National Competence Centres (NCC)**
 33. 08/07/2021. *1st COE-NCC Meeting*: First-principle simulations/quantum mechanical simulations in chemistry and materials science. Presentations by Elisa Molinari (MAX), Claudia Filippi (TREX) about activities and support actions from their respective projects. These included in particular: the development and support for applications codes; the use and/or development of software or middleware platforms; training offered for the related user communities.
 34. 01/09/2022. *2nd COE-NCC Meeting*: Presentation of EuroCC from Czech Republic and Austria. The NCCs presented to CoEs their activities, external interactions, and collaboration possibilities.
 - **Other events and activities.**
 35. 12/03/2021. *FocusCoE CoEs Co-Design Workshop* (online).
Session 1. "Different levels of co-design, where do CoEs come in?", panelist Fabio Affinito (Cineca)
Session 2. "Co-Design for new usage", panelist Leopold Talirz (EPFL).
 36. 23/03/2021. *FocusCoE workshop @ EuroHPC Summit Week 2021*¹⁵: Elisa Molinari (Cnr) and Joost VandeVondele (ETHZ) contributed to the FocusCoE live panel discussion moderated by Erwin Laure (MPCDF) on the status and future of Applications Support in EuroHPC.
 37. 09/2021. *FocusCoE Newsletter #12*, in the Introduction a detailed description of MAX.

¹⁵ <http://www.max-centre.eu/events/max-coe-workshop-ehpcsw21>



Deliverable D10.6
Final report on MAX in the European, national,
international HPC ecosystems

https://www.hpccoe.eu/?mailpoet_router&endpoint=view_in_browser&action=view&data=WzEwLCI4NjBmOGVhMWZmZGMiLDA5MCwwLDFdf

- 38. 26/10/2021. MAX and other CoEs, coordinated by FocusCoE, attend the EUSEW21 - EU Sustainable Energy Week (online). Elisa Molinari acted as panelist in “HPC and Big Data as key enablers of the Clean Energy Transition (panel with other CoEs EoCoE, MAX, HiDALGO, HVL, and FocusCoE) - Energy Talk 3795.
- 39. 12/2021. Collaboration to revision of the ETP4HPC Strategic Research Agenda, chapter on Applications.
- 40. 22/03/2022. Elisa Molinari attended the “European HPC CoEs: perspectives for a healthy HPC application eco-system and Exascale¹⁶”, a FocusCoE event with the EU CoEs @ EuroHPC Summit Week 2022.



Figure 13: Group photo @ EuroHPC Summit Week 2022 (E. Molinari is the second from left).

- 41. 04/2022. MAX collaborates to the definition of the “CoEs Impact brochure¹⁷” and of the “CoEs Service Booklet¹⁸”, launched on April 12, 2022.
<https://twitter.com/FocusCoE/status/1513857827718287374>

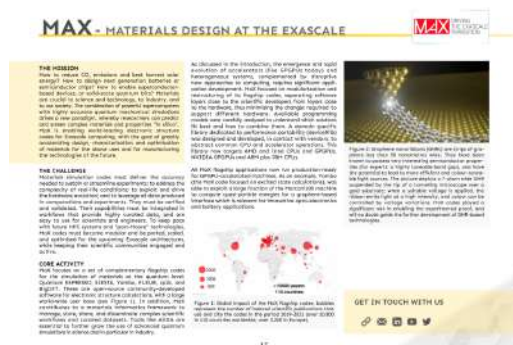


Figure 14: The FocusCoe Impact brochure and pages dedicated to MAX.

- 42. 02/06/2022. Workshop on Software Co-Design Actions in European Flagship HPC Codes (EU-SW-CODESIGN-22) @ ISC HP 2022, Hamburg (DE). Talk: Performance Assessment and Energy Efficiency of MAX Codes, Daniele Cesarini (CINECA)¹⁹.

¹⁶ <https://www.hpccoe.eu/2022/03/24/focuscoe-at-eurohpc-summit-week-2022/>
¹⁷ <https://www.hpccoe.eu/impact/>
¹⁸ <https://www.hpccoe.eu/download/>
¹⁹ https://www.hpccoe.eu/wp-content/uploads/2022/05/EU-SW-CODESIGN-22_abstracts.pdf