D10.3

First report on MaX in the European, national, international HPC ecosystems

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Contents

Executive Summary

This "First report on MaX in the European, national, international HPC ecosystems" offers an overview of the rich activity of MaX CoE as an actor of the HPC ecosystem at different levels, working to address technical and policy issues of pan-European relevance, and to help overcome the fragmentation of European HPC activities in applications.

We describe the interactions MaX had and is having with the different actors in Europe at the HPC level, where we work with the EuroHPC Joint Undertaking, the CoEs ecosystem and Focus CoE, EOSC, ETP4HPC - the European Technology Platform for HPC, EPI - European Processor Initiative, PRACE, and all the main actors playing a role in the HPC realm.

MaX plays a leading role in its specific domain of materials research, and has strengthened its long established collaboration with the relevant stakeholders: details on the activity with Psi-k network, CECAM, EMMC, Graphene flagship, Batteries and BIG-MAP initiatives, NFFA, MarketPlace, GO-FAIR, OptiMaDe are given, as well as some other relevant initiatives at national and international level.

1. Introduction

The first half of MaX life has coincided with a unique phase in the European HPC and data initiatives, with a strong increase in investments and the launch and construction of the EuroHPC Joint Undertaking. Applications represent one of the key pillars in its strategic agenda, and Centres of Excellence (CoEs) are now recognized as the pillars to maintain and strengthen the European leadership on applications in their respective domains.

MaX has been extremely active in the collaborative efforts that characterize this phase, primarily by performing all its technical work 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 D10.3.

In this deliverable 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 organizations and events. The effort required by these structuring activities has been larger than initially planned, but we consider it an investment towards the quality and impact of our future work.

For convenience, this deliverable is organized according to the main organizations with which we have been working, first within the general HPC ecosystem (Section 3) and then in the specific domain of materials research (Section 4). More details on collaborative initiatives of MaX with European institutions on training and education are given in deliverable D8.4.

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:

EuroHPC Joint Undertaking

- The main contribution of MaX to the success of EuroHPC is in the applications-oriented pillar and the cross-cutting co-design efforts that will be crucial for its overall success (see activities and deliverables of WP4).

  MaX will have codes and use-cases ready to run on all the pre-exascale systems as soon as they will be available (see activities and deliverables of WP1-4 and WP6), and has offered training for code developers and users (activities and deliverables of WP8).

  Concerning the pre-exascale EuroHPC machines, materials science and MaX codes have become one of the main focus areas for the Leonardo consortium for the hosting of a pre-exascale system.

- Concerning the coordination process, MaX has contributed with its CoE experience to shaping the EuroHPC policies on Applications and Training.

  Two leading MaX participants are members of the EuroHPC Research and Innovation Advisory Group (RIAG): Elisa Molinari (MaX coordinator) and Carlo Cavazzoni (WP4 leader). They have been especially active in the preparation of

- the Strategic Research and Innovation Agenda 2019 (https://eurohpc-ju.europa.eu/documents/EuroHPC_RIAG_Strategic_Agenda_2019.pdf)

- the Multiannual Strategic Research and Innovation Agenda 2021/2022 (in preparation, to be completed in June 2020)

  Molinari and Cavazzoni have directly contributed to the writing of the Sections and Recommendations on “Applications” and on “Training”, largely based on the experience of MaX.

  List of attended RIAG meetings: Brussels March 1, 2019; Brussels April 5, 2019, Poznan May 13, 2019; Brussels June 27, 2019; Barcelona August 29, 2019; Brussels October 10, 2019; Munich December 12, 2019; Brussels February 19, 2020; Online March 23, 2020; Online April 29, 2020. In addition, numerous sessions of informal RIAG working groups to prepare the RIAG meetings and recommendations.

- MaX has actively participated in the main meetings and dissemination events (co-)organized by EuroHPC:

- the European HPC Summit Week 2019 in Poznan (May 13-17, 2019) with Carlo Cavazzoni (CINECA) presenting “Grand challenge applications: technical requirements for the exascale era” during the Co-Design Workshop (May 15, 2019) https://twitter.com/max_center2/status/1128916892046045185 and Sebastiaan Huber (EPFL) representing MaX in the 1st European Communities Workshop on Exascale Computing Focus on High Performance Data Analytics - Session 1 – CoEs & HPDA (May 16, 2019) https://twitter.com/max_center2/status/1128983536449544193

Figure 1. EHPCSW Poznan 2019 group picture. From MaX E. Molinari, L. Neri, C. Cavazzoni, F. Magugliani.

- HPC Policy + Digital Excellence Forum in Helsinki (September 19, 2019) with Molinari presenting the European HPC ecosystem in the plenary panel session (https://twitter.com/max_center2/status/1174591203700031489)

- In addition, a special MaX session "Computational Materials Science towards the Exascale: performance portability and use cases" was organized in the frame of the EuroHPC Summit Week 2020 in Porto (March 24, 2020): https://events.prace-ri.eu/event/937/timetable/?view=standard: unfortunately the whole meeting was canceled due to the Covid outbreak, so the session will be rescheduled.

CoEs ecosystem and Focus CoE

- Specific collaborative interactions have involved MaX and other CoEs: in particular with POP on profiling, with eCAM on the development of modules in the Electronic Structure Library and on some training events (see D1.3 and D8.2), and with Bioexcel on possible contributions of MaX QM codes in biomolecular simulations.
- Here we mention the management contributions towards establishing a broader lively and effective coordination among the CoEs. MaX has contributed to establishing the HPC CoE Council - HPC3, which involves the Directors of all CoEs and now meets regularly to discuss common issues, and participates in its leading team (https://www.focus-coe.eu/index.php/2019/06/12/hpc-coe-council-established-at-ehpcsw/) and in many joint initiatives. Even if MaX partners are not beneficiaries of the Focus CoE CSA (https://www.focus-coe.eu), several MaX representatives have contributed significantly to its different WPs: Elisa Molinari (Vice Chair of the HPC CoE Council - HPC3), Luisa Neri (HPC3 & WP3 CoE Industry Interaction), Silvana Muscella and Francesco Osimanti (WP3 CoE Industry Interaction and WP 5 Communication, dissemination and outreach), Elisabetta Narducci (WP3 CoE Industry Interaction), and Daniele Varsano (WP4 Training).

  Among the joint initiatives, we point out the systematic coordination of training activities among the CoEs and with other stakeholders. MaX representatives (Daniele Varsano & Maria Celeste Maschio) have actively participated in the European HPC Training Stakeholder Workshop organized by FocusCoE in Brussels on October 8, 2019 to design and coordinate future training activities.

  Moreover, MaX delegates are involved in the HPC3-WP3 working group which is devoted to sustainability. All the CoEs are making a common effort, sharing views and practices, in order to draft a sustainability program to present to the Commission for the years to come.

  List of main FocusCoE meetings and events attended by MaX personnel:

  - HPC3 (council) meetings: 21/02/2019 Kick-Off meeting in Frankfurt (DE), 13 & 17/05/2019 in Poznan (PL) at EuroHPC Summit Week, 12/06/2019 (telco), 10/07/2019 (telco), 04/09/2019 (telco), 09/10/2019 (telco), 15/11/2019 (telco), 17/12/2019 in Luxemburg, 12/02/2020 (telco), 26/3/2020 (telco), 13/5/2020 (telco);
  - HPCR Sustainability: 18/02/2020 (telco), 13/03/2020 (telco);
  - WP3 Industry interaction: 12/07/2019 (telco), 19/09/2019 (telco), 12/12/2019 (telco), 20/03/2020 (telco);
  - WP4 Training: 8/10/2020 in Brussels (BE), 28/04/2020 (telco).

- MaX has been an active participant in the following meetings organized by the EC for CoE coordination:
- Centers of Excellence on HPC Applications Workshop (Brussels, December 3, 2018)
- HPC CoEs Cluster meeting (Luxembourg, December 18, 2019)

EOSC

MaX and EOSC have set up a strong collaboration, thanks to S. Muscella (Trust-IT, WP9 leader) playing a leading role in EOSC as the High Level Expert Role Group chair, and to G. Pizzi (EPFL, WP5) leading all the MaX technical contributions.

The collaboration milestones are as follows:

- EOSC and EOSC-Hub collaboration setup (online meeting on 19/02/2019 defining guidelines for the further collaboration). The collaboration actions are at the technical level (MaX WP5: AiiDA, Materials Cloud (Archive), AiiDA Lab) and at a more general level including training, services and industrial engagement through Digital Innovation Hub;
- Participation in the EOSC-hub week (10-12/04/2019 Prague). Invited talk by Giovanni Pizzi (EPFL) representing MaX CoE at the HPC centres of Excellence section where MaX was presented as a pilot case: "Pathways for EOSC-hub and MaX collaboration. A platform for reproducible science with full provenance" (April 11, 2019)
  https://www.eosc-hub.eu/sites/default/files/2019_04_PIZZI_MaX-AiiDA-MaterialsCLoud-EOSC-Prague.pdf
  G. Pizzi's slides:
  https://www.slideshare.net/TheEOSChubproject/pathways-for-eoschub-and-max-collaboration

Figure 2. Giovanni Pizzi and the MaX-EOSC presentation (source Twitter https://twitter.com/max_center2/status/1121752261833777152)

- Collaboration for the EOSC survey (February 2020) for the realization of the booklet "Advancing engagement between HPC Centres of Excellence & EOSC" available at https://zenodo.org/record/3727821#.Xn3AkNNKhQJ

- Active collaboration and integration with the EOSC Marketplace portal: notably, registration of the MaX service "AiiDA lab" on the EOSC Marketplace (https://marketplace.eosc-portal.eu/services/aiida-lab)
- Integration of the AiiDA lab authentication with the EGI Check-In authentication service, to allow secure login by any researcher with an academic affiliation with their institutional credentials (https://marketplace.eosc-portal.eu/services/aiida-lab)
- Participation to the EOSC Hub Early Adopter Programme, to obtain virtual resources (via kubernetes) to run a fully-scalable AiiDA lab infrastructure supporting 100+ users (https://eosc-hub.eu/research-communities/open-aiida-lab-platform-cloud-computing-materials-science); grant awarded and service to be launched in the summer of 2020.

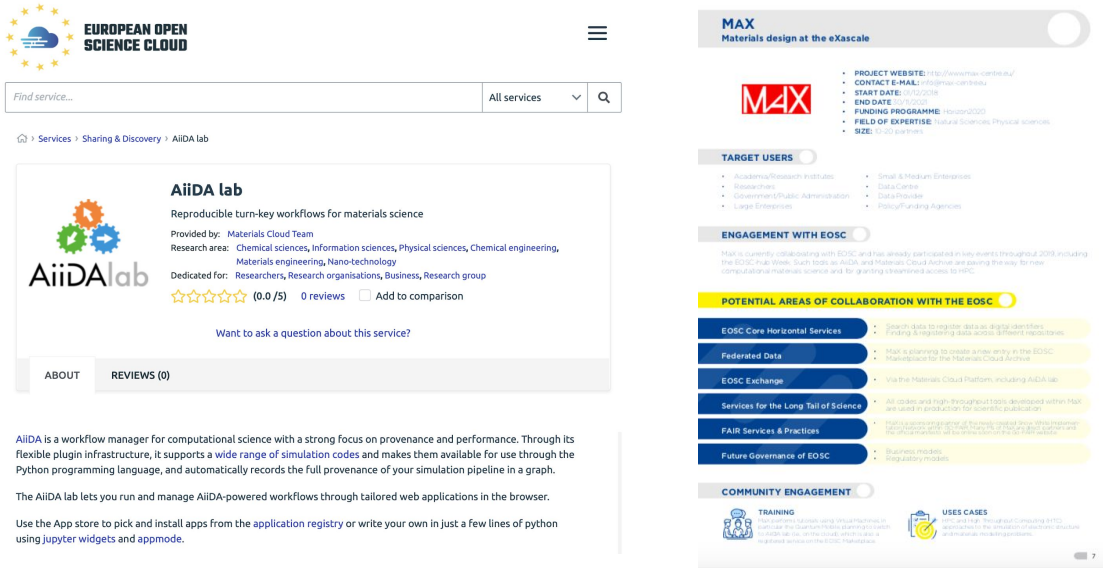


Figure 3. (Lefy) AiiDA lab service page on the EOSC hub Marketplace catalogue. (Right) MaX page in the European Science Cloud Catalogue

ETP4HPC - the European Technology Platform for HPC

MaX has contributed to several goals of Strategic Research Agenda (SRA) of the ETP4HPC in different areas, especially with the activities of WP4 (see D4.3 and D4.4).

MaX partners who are leading members of the ETP4HPC (among them C. Cavazzoni, F. Magugliani) have been active in shaping the new SRA, especially the parts on Applications, largely taking into account the lessons learned in MaX.

As a specific MaX contribution to the SRA 4 of ETP4HPC (https://www.etp4hpc.eu/sra.html), Andrea Ferretti represented our CoE, provided contents for this key deliverable and contributed to the final document.

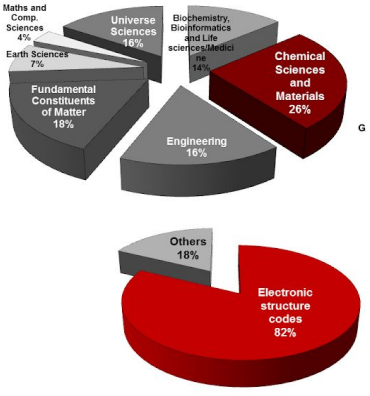
EPI - European Processor Initiative

MaX has been collaborating with EPI systematically on common co-design initiatives, communicating findings about MaX codes and co-design vehicles (mini-apps, libraries): in particular, EPI has adopted LAXlib miniapp from Quantum ESPRESSO and DBCSR library from CP2K, as well as BigDFT application. Together with ARM, in MaX we have then performed preparatory work to validate the codes and mini-apps on ARM architecture and deliver performance evaluation on simulated and emulated SVE instruction set. Then we have shared profiling information with EPI, in particular for what concerns typical matrix sizes used in linear algebra modules and libraries. This information will be used in EPI to assure the vectorization level available in the future EPI processor as well as the size of the different chase levels will be adequate for MaX applications. From some preliminary tests that we have done on real ARM processors with SVE (made available to MaX through Cineca by Fujitsu) the performances are encouraging and no major bottlenecks with respect to the memory, cache, and vectorizations are present.

PRACE

MaX has actively participated in a number of coordination meetings involving Prace, including the PRACE-CoEs-FET HPC-EXDCI Workshop (https://events.prace-ri.eu/event/750/), specifically aimed at boosting interaction between Prace, CoEs, and the community. Specific 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);
- collaboration with work packages dealing with codes, benchmarks and libraries: some of the MAX codes are included in the PRACE benchmark suite;
- coordination of MaX high level domain specific training with training actions offered by PRACE, and specific contributions from MaX in joint events with PRACE as the “AiiDA Hackathon developing code plugins and robust scientific workflows” held in Bologna in February 2020;
- participation in an industrial engagement event “HPC for Industry 4.0 @Cineca”, Milan, May 21-23 2019 (https://events.prace-ri.eu/event/834/) where E. Molinari presented “MaX: screening and designing materials with HPC”.



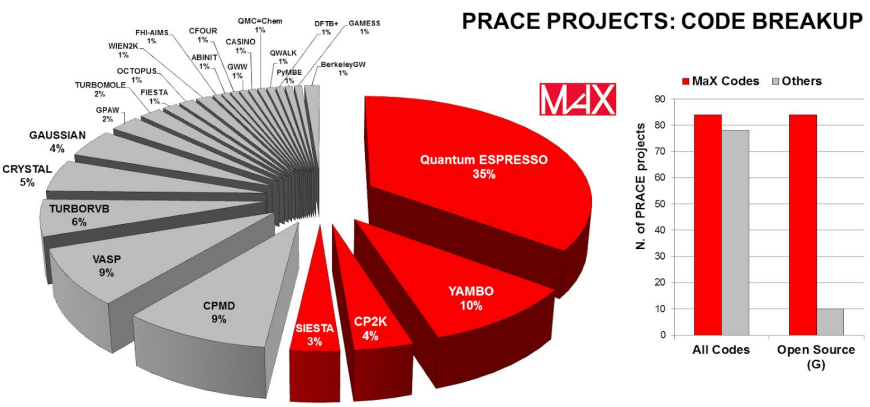


Figure 4: According to PRACE data (calls from 1 to 15), European codes in the materials domain are leading. Examples of data that refer to the number of PRACE granted projects using a given code, within the 'Chemistry and Materials Science' domain. Only 'electronic structure-based' codes are considered in this slide.

Source: MaX elaboration from Prace data, 2019.

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

Computational research on materials is one of the major users of HPC resources in Europe and worldwide. The whole of MaX is committed to enabling the materials research community to make the best and broadest use of advanced HPC at the (pre-)exascale, especially in Europe. This is done primarily by developing the MaX codes and the data ecosystem (see WP1-3 and WP5 activities and deliverables) and providing advanced training and user engagement (see WP7-8 activities and deliverables).

Within WP10, we report on MaX activities to strengthen collaborations with communities in Europe that can best take advantage of the above developments and of the future EuroHPC supercomputers, and with communities worldwide which are/can be users/developers of MaX codes thereby enhancing their impact.

MaX has invested significant resources on collaborative initiatives with European institutions on training and education. More details on these are given in D8.4.

Psi-k network

Psi-k (https://psi-k.net) 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 organization 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 is the chair and several MaX partners are members of the Scientific and the Trustees boards), and has established structured collaborations aimed at disseminating MaX results in the scientific community and engaging prospective users:

- co-organization and support of several specialized workshops;
  * Tutorial on writing reproducible workflows for computational materials science, May 21-24 2019, EPFL, Lausanne (CH). MaX Organizers and speakers: L. Talirz, S. Huber, A. García, A. Ferretti, S. Cottenier, G. Pizzi.

  * Computational School on Electronic Excitations in Novel Materials using the Yambo code, January 27-31 2020, ICTP Trieste (IT). Max Organizers and speakers: S. Baroni (SISSA), A. Ferretti, A. Marini, D. Sangalli, D. Varsano.

* E-CAM Extended Software Development Workshop: Integration of ESL modules into electronic-structure codes, February 17-28 2020, CECAM-HQ-EPFL, Lausanne (CH). Organizers: E-CAM, CECAM, Psi-K, MaX. MaX speakers: A. Garcia, S. De Gironcoli.

- participation in the design and organization of the Psi-k-2020 conference (initially planned for September 2020 in Lausanne, now rescheduled to August 2021, due to COVID-19 emergency): specific MaX contributions will include a dedicated booth, the organization/participation/chair in several thematic sessions, a specific MaX event after the conference closure;

- dissemination of MaX openings and events through the Psi-k mailing list.

List of main coordination meetings with Psi-k: Lausanne October 21-22, 2019; Paris November 21, 2019; teleconference May 22, 2020.

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 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 strategy and policy discussions together with CECAM. Important examples are

- the "CECAM brainstorming event on Data driven Science" held in Lausanne on March 25-26, 2019, gathering experts in order to address different challenges of this area, including infrastructure, dissemination, data analysis, intellectual property and ownership of data, and development of new methods. A considerable part of the discussion was to identify needs and actions ahead in the short, medium and long term, together with the main stakeholders in Europe. Giovanni Pizzi (WP5) presented the activities and plans of MaX; Bluegel, Cavazzoni, Ordejon attended and contributed to coordination;
- the celebration and brain-storming event "Molecular and materials simulation at the turn of the decade: Celebrating 50 years of CECAM" Lausanne, September 9-12, 2019: several MaX members give very prominent scientific talks, and Molinari participated in a policy panel discussion on the future of the scientific domain.

Importantly, MaX has established a structured collaboration with CECAM, especially aimed at collaborative training events:

- co-organization and support of several schools;

  * Picking flowers: Hands-on FLEUR, September 9-13, 2019, Forschungszentrum Jülich, Jülich (DE). Organizers: Forschungszentrum Jülich, MaX. MaX speakers: D. Wortmann, U. Alekseeva.

* E-CAM Extended Software Development Workshop: Integration of ESL modules into electronic-structure codes, 17-28 February 2020, CECAM-HQ-EPFL, Lausanne (CH). Organizers: E-CAM, CECAM, Psi-K, MaX. MaX speakers: A. Garcia, S. De Gironcoli.

* Digital Learning for Electronic Structure Theory Codes, scheduled for April 27-30, 2020 was postponed to a future date due to COVID-19 emergency. A one-day online event titled Digital Learning after its Black Swan was organized on April 28, 2020. *Organizers:* UGE, MAX, CECAM. MaX speakers: S. Cottenier (UGE), G. Pizzi (EPFL).

* Summer School on Advanced Materials and Molecular Modelling with Quantum ESPRESSO, JSI, Ljubljana (SLO). September 16-20, 2019. Organizers: QE foundation, MAX, Jožef Stefan Institute, CECAM. MaX Speakers: S. Baroni (SISSA), P. Giannozzi (UniUd), P. Delugas (SISSA), G. Pizzi (EPLF), C. Cavazzoni (CINECA), P. Bonfà (Cnr).

EMMC

EMMC, the The European Materials Modelling Council, is an organization promoting materials modeling with focus on industrial research and innovation. Initiated as a CSA, since 2019 it has evolved into the EMMC ASBL Association (https://emmc.eu). MaX has been collaborating with both entities especially to promote MaX codes in the context of multi-scale approaches towards industrial end-users.

Within this collaboration, for example:

- Molinari has delivered a plenary presentation of MaX at the EMMC-CSA Workshop on Industrial impact of materials modelling (Turin July 8-10, 2019: https://emmc.info/events/emmc-torino2019/).
- the EMMC Executive Secretary, Gerhard Goldbeck, gave a presentation within the MaX webinar on “Industry and materials design at the exascale: bridging the gap” (September 4, 2019:https://cordis.europa.eu/article/id/125731-industry-and-materials-design-at-the-exascale-bridging-the-gap).

Graphene flagship

MaX has established a new collaboration with the Graphene Flagship, with the aim of ensuring the best use of its codes and ecosystem within that community. The reason is that a significant component of the flagship --both from industry and academia-- is already performing materials simulations, representing a potential users basin of the next EuroHPC supercomputers. It is thus important to support this transition and the uptake of best practices and codes.

After many informal meetings, we have organized a MaX-Graphene flagship joint initiative during the Graphene Week 2019 in Helsinki on September 24, 2019 (http://graphene-flagship.eu/grapheneweek/editions/GrapheneWeek2019/Pages/default.aspx).

The event consisted of

- a Graphene Flagship – MaX joint workshop on “High-performance computing for 2D materials research”, with a Parallel Session on Tuesday, 24 September 2019 (15.30-18.00) and a Poster Session (18.00-20.00)
  Chairs: Elisa Molinari – director of MaX Center, Vladimir Falko – Director of NGI

- a policy session: “European HPC initiatives and 2D materials research: collaborating and funding opportunities” on Tuesday, 24 September 2019 (14:30-15:30) chaired by Nicola Marzari with a presentation by Elisa Molinari and open debate.

The workshop engaged computational scientists, active in the graphene community around the following topics: Modelling of complex 2DM systems: interfaces, nanostructures, hybrid structures; Properties of novel 2DM: expanding the set of properties that can be predicted; Development of efficient computational approaches optimized for 2DM modelling; High throughput computation and automated data analysis in 2DM research. The discussion focused on the HPC and HTC challenges and the support that MaX can offer to this user community.

https://graphene-flagship.eu/grapheneweek/editions/GrapheneWeek2019/Pages/HPC-Workshop.aspx; http://www.max-centre.eu/news/max-graphene-week-2019.

Figure 5. Pictures from the Graphene Week 2019, E. Molinari’s talk.

Batteries and BIG-MAP initiatives

Research on future batteries is a huge field for computational materials simulation and design. Most of the current work, however, is not taking full advantage of HPC capabilities. MaX has established a close collaboration with the team working towards the Battery2030+ initiatives (including its large industrial component), to ensure the best use of MaX codes and EuroHPC ecosystem within that community. As future work will focus on automated materials design (https://battery2030.eu/research/research-themes/accelerated-discovery-of-battery-interfaces-and-materials-/), MaX has been working to strengthen the HPC and HTC contribution in that context.

As a result, MaX has participated in designing a large proposal entitled BIG-MAP "Battery Interface Genome - Materials Acceleration Platform" (GA 957189), which has been funded within the H2020-LC-BAT-2019-2020 call. 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. The BIG-MAP consortium includes 21 leading European partners (20MEuro) with complementary battery skills and essential competence from critical research areas such as quantum machine learning, deep learning and autonomous synthesis robotics. MaX will coordinate the HPC and HTC effort of BIG-MAP through its partners CNR, CSIC, EPFL.

Discussion meetings with the battery community include: Copenaghen January 18, 2019; Copenhagen September 5-6, 2019; Copenhagen December 6, 2019, and many other bilateral and informal discussions.

NFFA

MaX members (CNR, EPFL) provide computational simulations and data stewardship within the H2020 NFFA (Nanoscience Foundries and Fine Analysis) project, and in particular in the "Theory and simulation installation" (https://www.nffa.eu/offer/theory-simulation/) and in a Joint Research Activity on "e-Infrastructure for data and information management".

MarketPlace

MaX members (EPFL) provide the data and model services - through AiiDA workflows - for the H2020 MarketPlace project, GA 760173 (https://www.the-marketplace-project.eu). This project is developing a "materials modelling marketplace" to boost industrial innovation by collecting, adapting and integrating modelling components from different academic and industrial communities to provide a single point of access, through an on-line gateway, for the many materials modelling activities in Europe.

GO-FAIR

MaX is part of 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). As such, it is committed to implement clearly defined plans and deliverables to implement an element of the Internet of FAIR Data and Services (IFDS), foster a community of harmonized FAIR practices, and communicate on critical issues on which consensus has been reached and which are of importance for the community.

OptiMaDe

MaX members are part of the OptiMaDe consortium of worldwide computational efforts dedicated to make materials databases interoperational by developing and adopting a common REST API, whose specifications are regularly updated and approved by all members - currently in v1.0-rc1: https://github.com/Materials-Consortia/OPTIMADE/blob/master/optimade.rst.

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 supported up to 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.

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 2014-2020), which is supporting the uptake of MaX codes and their application to a few use cases of industrial relevance.

Materials and Molecular Modelling (MMM) Exascale Design and Development Working Group (DDWG), UK

MaX supported this working group to design and submit a proposal for HPC activities in the UK, using interesting codes and MaX libraries. The application was successful and the project has just started on May 1, 2020.

Third-country initiatives

Concerning third-country initiatives, MaX has continued to interact with similar Centres on Materials design worldwide. The initial idea of organizing a second meeting of the Directors, similar to the one held in Paris in 2017 (https://paris-meeting-2017.uchicago.edu/#about), has been postponed and will likely take place at the Psi-K2021 conference in Lausanne.

Close interactions have meanwhile been strengthened with the **computational materials centers 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 Study of Excited-State Phenomena in Energy Materials. These close interactions provide optimal synergies between the US activities and the MaX efforts. In addition, Marzari was hosted in 2019 for his sabbatical in the Center for Computational Quantum Physics in the newly formed Flatiron Institute in New York City.

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. In addition, he is part of the International Advisory Board for the African MRS (Materials Research Society) that will be held in Kigali (Rwanda) in 2021. In this context, two Schools have seen significant contributions from MaX: the 1st Central African School on Electronic Structure Methods and Applications (CASESMA) Dschang, Cameroon, November 18-23, 2019; and the Eastern Africa School on Electronic Structure Methods and Applications, Addis Ababa, July 1-5, 2019. (For more information on these training events see deliverable D8.2.)

In addition, we point out the important

Collaboration with RIST (Japan)

RIST -- Research Organization for Information Science and Technology -- is a general incorporated foundation working in Japan for the development and utilization of computational science and technology to support a highly information-oriented society (http://www.rist.or.jp/ehome.html).

A MaX team with Quantum ESPRESSO developers, ARM and Cineca representatives, after a meeting occurred at SC19 (SuperComputing19, Denver (US), November 17-22, 2019), have started a collaboration with a RIST team working in the porting and optimization of Quantum ESPRESSO in future Fugaku pre-exascale Japanese machine. This is because Quantum ESPRESSO is one of the most used applications in the Japanese network of supercomputers as well. A face-to-face meeting with RIST representatives occurred in January 2020, in Bologna, where they illustrated the level of support they are going to dedicate to Quantum ESPRESSO and then contributing with feedbacks about bottlenecks and solutions they will find for the Fugaku system, that will be about half exaflops. The MaX team on the other hand offered support and collaboration since these activities will be extremely important for the EPI processor as well. EPI in fact will share the base architecture (ARM) and SVE with the Fujitsu AFX64 processor of Fugaku. In a way, porting on Fugaku will be a sort of warm-up for the porting on future European Exascale systems.

4. Conclusions

The main contribution of MaX to the European and international ecosystem comes undoubtedly from the work of our 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.

In the present deliverable we have shown how such contributions have been constantly accompanied by an effort to elaborate joint European strategies and policies 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 organizations and events.

MaX is now recognized as one of the cornerstones of the European application and HPC ecosystem, and as a reference point for the computational materials research community in Europe and beyond.

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.