



## D8.1

# Training and Education Programme

Daniele Varsano, Maria Bartolacelli, Maria Celeste Maschio

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**Authors:** Daniele Varsano, Maria Bartolacelli, Maria Celeste Maschio

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## D8.1 Training and Education Programme

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## 1 Executive Summary

The deliverable 8.1 is centered on the plan of specialised training and education in computational materials science. In order to train the new generation of both developers and code users, MAX will offer different and dedicated events structured as workshops, courses, tutorials, schools and hackathons. A special attention will be dedicated to the training of the users of MAX flagship codes with a focus on best practices and efficient use of the codes in pre-exascale machines; training on new developments coming from the efforts towards the exascale enabling (WP1) and algorithmic advances (WP3) will also be included. A particular attention will be dedicated to training young people and women working in scientific and technological research.

The purpose of the Education and Training plan is to reach a wide community, both in academia and industry, offering a domain-specific training program at pan-European level. To this aim, MAX CoE will coordinate most of these training activities in collaboration with CECAM, Psi-k and ICTP, benefitting from the established tradition and user-base they have in the education domain and contributing to widening the engagement of different communities. The partners in charge of this WP are **CNR**, SISSA, ICN2, CEA, EPFL, Juelich, ICTP, UGE.



## 2 Introduction and Objectives

MAX devotes an important amount of resources and efforts to increase the number and proficiency of scientists and industrial users interested in computational methods and in the optimisation of applications. Particularly, a rich training offer will be presented to the new generation of code developers and scientists in computational materials research. Moreover MaX will coordinate, contribute and integrate its proposal with other transversal European initiatives.

Among the actions that MAX will put in place in order to pave the way for the transition to the exascale technologies, the attention to the education and the needs of the user communities is one of the most important. The aim of MAX activities is hence to widen the pool of competent users **at pan-European level, both in academia and in industry**, filling the skill gaps and favoring the full deployment of European potential in this field.

WP8 is dedicated to the computational materials community, fostering the know-how transfer to both developers and users. In general, MAX will plan hands-on course on MAX flagship codes and their developments produced in the CoE, releases of related documentation and materials as well as training events towards new developers.

The training and education activities supplied will then create a new generation of expert developers and users, through effective partnerships with European educational institutions. A key objective in MAX actions will be ensuring a continued and updated training, in order to provide a dynamical framework for the educational requirements. The research and development staff will be fully supported, guaranteeing the objective of evolution of MAX activities and tools.

Like in the first phase of MAX, the key training priorities will target an appropriate education, spanning in the different levels of user knowledge, and a real effectiveness, monitoring the user know-how uptake and the post-activity evaluation of user satisfaction. All the activities will be also guided by the attention toward the inclusivity and the gender balance principles. Finally, the MAX tools and training products will be the result of a transparent process, where all scientists and organisations involved will be aware of the realization pathway and the funding sources. Such hallmark will make MAX resources highly trustworthy for all the stakeholders and end-users.

MAX plans to organize a series of diversified initiatives that can be summarized in the three different tasks of the WP:

T8.1: Training devoted to fill the pipeline of new generation of code developers. This task includes specialized hands-on courses to provide state-of-the-art technical know-how. In



practice this task will be developed in close connection with WP1, WP2 and WP3, by organizing:

- courses focusing on strategies and implementations of recent advances towards a better exploitation of the forthcoming (pre-)exascale architectures in MAX codes and domain specific libraries. This action includes also workshops concerning new algorithms and developments produced in the CoE;
- hackathons and coding days/weeks to improve MAX codes and domain specific libraries. The events will bring together new developers, principal developers of the CoE codes, developers of codes outside the consortium, and experts in HPC programming and accelerator technologies;
- training through research in MAX labs, offered to new developers that are interested in specific implementations in flagship codes. Academic users could take advantage of the established MAX collaboration with HPC-Europa3 programme.

T8.2: Advanced training for academic and industrial users devoted to broadening the pool of scientists in computational materials science and fostering a large and efficient use of (pre-)exascale HPC codes in the EU. We will do this by a combination of traditional and contemporary education actions, paying special attention to lowering the threshold for young researchers and companies. In practice we will implement this task by:

- organizing schools in the domain of materials science, with emphasis on the new capabilities of electronic structure codes enabled by the (pre-)exascale machines. These events will typically include an introduction to concepts and methods, and a code-specific or code-group-specific hands-on training for both new and experienced users;
- developing flexible teaching modules aimed at Master/PhD students and university teachers, on frontier computational methods within their domain (e.g. computational materials science, computational physics, computational chemistry, etc);
- one-on-one training by hosting academic and industrial researchers in CoE laboratories, for training/collaboration visits on scientific projects involving the use of MAX flagship codes. Academic users can take advantage of the collaboration of MAX with the HPC-Europa3 programme.

T8.3: in the pan-European context, MAX will give relevance to every chance of coordination and contributions to transversal training initiatives. For this reason, domain specific content will be provided to coordinated initiatives, which will be organized with PRACE and the FocusCoE CSA, or in collaboration with other CoEs. This includes design of training activities, scientific and technical content, lectures and training materials. As there is a targeted interest in software development techniques aimed at (pre-)exascale systems, MAX will largely contribute to training initiatives organized by HPC centres and PRACE. The offer will include domain-specific content and integrated "materials-specific sessions" produced within the CoE, oriented to all the user levels.



### 3 Strategy

The provision of training activities given by MAX is prepared in order to cover the main aspects of computational materials science of interest for the end-users and the software developers. The planned actions by MAX will be tailored on the specific needs of each kind of audience, through specific formats. In particular, the promotion of such actions toward young researchers and women will be fostered. The audience is mainly composed by:

- software developers;
- academic researchers;
- industrial researchers;
- master and PhD students

and hence the main developed formats are:

- domain specific courses on pre-exascale strategy and implementation, complementary to PRACE and FocusCoE activities;
- hackathons and coding days/weeks dedicated to MAX flagship codes and domain specific libraries;
- highly specialized training hands-on tutorials on flagship codes and workshops on new algorithms and methods produced in the CoE;
- training for visiting researchers in MAX labs;
- courses on HPC in Materials science for Master and PhD students, considering also the production of online modules with reusable content for self-paced skill development. By conceiving these modules from the start as online modules suitable for self-paced study as well as for use with a local teacher, they will naturally evolve to course material that can be adopted by universities world-wide.

In the occasion of schools and workshops, high-quality recordings of the key lectures will be offered on a permanent basis in a dedicated section of the MAX website in order to reach many potential end-users who need training at a moment when no relevant school is available.

For the whole period, MAX will devote a notable effort to assess the general guidelines leading the educational actions made by the CoE, guaranteeing a harmonic framework for the available offers.

In the first months of the MAX activities, a dedicated training working group, including at least one person from each node active in training activities, has been identified. The working group is meant to discuss the training events and monitor the status of the organization of the events by meeting on a regular basis by teleconference. In this first period of MAX, the working group has started to organize several events (see Sec. 5) and has defined strategies and guidelines for the MAX training program. The working group has also identified a *team for Hackathons organization* coordinated by ICTP, composed by code



developers and experts from supercomputing centres. The aim is to coordinate at the best the events of T8.2 meant for training the young code developers. This task will be developed in a tight interaction with WP1, WP2 and WP3. Strategies and guidelines to achieve the training MAX objectives include the following actions:

- In order to widen the action of MAX and extend the pool of competent users **at pan-European level, both in academia and in industry**, MAX will organize some events in collaboration with Institutions of countries outside the Consortium and whenever possible the location will be chosen inside such States to additionally foster local users presence (see events n. 3, 4, and 7).
- **MAX will foster interactions and synergies with other CoEs and EU infrastructures:** this includes participation of MAX members in training events in collaboration with other CoEs (e.g. EoCoE, e-CAM, Bioexcel) or EU initiatives (e.g. Graphene Flagship, NOMAD, EOSC).
- **MAX will organize together with CECAM** at least 6 events among schools, workshops and hackathons. These events will be part of the CECAM program and will appear on the CECAM web page for flagship events and on the CECAM poster of activities. The synergy with CECAM will be instrumental in the engagement and participation of the community at large, by their involvement in scientific, training and outreach activities, including specialized workshops and hackathon events.
- **MAX will organize User-focus groups sessions** in the training events: since MAX arises as a user-driven CoE, the training actions represent an opportunity to collect input from the participants. In particular, user-focus group sessions will be included in the programme of all the events where it is recommended to have a fruitful interaction with the user (e.g. training on the use of flagship codes in HPC environments) (e.g. Events 5 and 6). The main emerged messages, as specific user needs and advice on the best use of a certain code for a particular scientific problem, will be collected in a report and shared with the relevant MaX teams.
- **Feedback form in MAX training events:** all the actions in this framework will have a form, an anonymous evaluation and satisfaction questionnaire that the attendees will be asked to compile at the end of the events. From this final document and the initial subscription form, accurate statistical data will be collected to provide measurable impacts of MAX training events.



- **Use of the Quantum Mobile:** the use of this powerful MAX product is strongly encouraged in tutorials and hands-on sessions, in coordination with the developments made by WP5 (Quantum Mobile) and WP7 (containers).
- **Online training material:** tutorial texts and other training material will be available online through recorded video lectures. Such materials will be stored in MAX dedicated channels interlinked with the main MAX website. Moreover a dedicated training event (see event n. 15) will be devoted to “Digital Learning for Electronic Structure Theory Codes” meant to train the participants in developing professional online modules on HPC in Materials Science and tutorials for flagship codes.
- **Communication:** In close contact with WP9, MAX training events will be properly promoted and advertised *via* the MAX communication channels. The organizers of the planned events will be in charge of communicating to the WP9 all the useful information about the event that will be published in the MAX website. The WP9 then will be in charge to properly promote the event through news, mailing lists and social media channels.
- **Visiting researchers in CoE laboratories:** as extensively experimented in the previous phase of MAX, academic and industrial researchers may be hosted and trained in MAX labs. The visits may be related to collaborations involving MAX flagship codes and hands-on training. The academic users can take advantage of MAX collaboration with HPC-Europa3 programme. This activity is already in place and 16 researchers have been hosted in our labs since the beginning of MaX (December 2018).
- **Industry participation:** the industrial involvement is highly important for MAX CoE. To achieve this goal, a constant effort will be done to provide a tailored training toward industrial users, and include them since the beginning in the audience of generic training events. Main industrial targets are independent software vendors, hardware companies and technological industries interested in the use first principle materials science codes and potential user of the MAX flagship codes (see events n. 3, 4, 6, 12, 13 and 15).



#### 4 Planned events over the course of MAX

In this section, the events organized and co-organized by MAX CoE following the above mentioned guidelines are described. At the time of writing this plan, the events taking place in the next year are typically well defined, details for the following period will be decided/finalized in the next months.

Learning will be in general achieved through lessons and presentations given by MAX experts and invited experts. In particular, to maximize the engagement of the computational community present in Europe and beyond, several events will be organized in collaboration with community organizations (especially CECAM and ICTP), profiting of the experienced contributions from the MAX developing teams and from the HPC computing centre experts.

##### **Specific training Workshops and Schools**

The actions described and listed below are dedicated to scientists in materials science field, covering different levels of background and giving particular emphasis on hands-on sessions. The aim is to provide technical knowledge in the field to young researchers, with a particular care in involving numerous women in science. This task will be coordinated by MAX WP6, in particular the CNR, ICTP and EPFL nodes.

- ❑ **1. Tutorial on writing reproducible workflows for computational materials science** organised by MAX (EPFL and CNR nodes) in Lausanne (May 21-24, 2019) with the support of Psi-k. Designed for Master and PhD students and Postdocs, the tutorial will introduce the state-of-the-art in workflow management and high-throughput computations by experts in the field, and will give participants in-depth hands-on experience using a tool that they can directly apply to their own research. URL: <http://www.aiida.net/news/tutorial-writing-reproducible-workflows/>
- ❑ **2. Picking flowers: Hands-on FLEUR** organised by MAX (Juelich node) at Forschungszentrum Juelich (September 9-13, 2019) with the support of CECAM. This tutorial focuses on training the participants in using our all-electron FLAPW DFT code FLEUR. In extension to similar previous tutorials, it also addresses the usage of FLEUR within the AiiDA infrastructure to build automatic work-flows applicable to materials screening applications. URL: <https://www.flapw.de/site/handson>
- ❑ **3. Summer School on Advanced Materials and Molecular Modelling with Quantum ESPRESSO** organised by MAX (SISSA node) together with the Jožef Stefan Institute of Ljubljana involving organizers from Ruđer Bošković Institute, Zagreb and the Institute of Physics of Belgrade. It will be held in Ljubljana, Slovenia, (September 16-20, 2019)



with the support of MAX and CECAM. Oriented toward students, postdocs and other researchers, the school will cover basic concepts as well as recent advances in materials science, with emphasis on DFT based methods and high performance computing. URL: <http://qe2019.ijs.si/>

- ❑ **4. A school on first-principles simulations of materials with SIESTA** organised by MAX (ICN2 node) in collaboration with the University of Belgrade (Serbia) in Belgrade (November 4-9, 2019) and the Barcelona Supercomputing Centre, with the support of CECAM. The school is aimed at students and researchers from different disciplines in materials science who already use, or plan to use, first-principles techniques to simulate electronic properties of materials. The students will learn the essential theoretical foundations, and to how to use the SIESTA code effectively (parallelization and new, more efficient, solvers). Pre- and post-processing tools will also be presented. Advanced features, such as the computation of quantum transport using the non-equilibrium Green's function approach will be introduced. Users from industry (Zepter International, Antonov d.o.o) will attend the school.
- ❑ **5. Computational School on Electronic Excitations in Novel Materials using the Yambo code** organised by MAX (CNR and ICTP nodes) at ICTP in Trieste (winter 2020) with the support of MAX, Psi-k and ICTP. The school introduces the students to Many Body Perturbation Theory approaches for calculation of electronic and optical excitations in novel materials. Theoretical lectures will be followed by hands-on based on the Yambo code to perform calculations on computer facilities for HPC. The focus of the school will be on accurate excited state calculations in solids and nanostructures, including non-linear optics and real time spectroscopy. In the last part of the school it is planned a user-focus session where the participants will directly interact with teachers and developers on specific capability and setting for HPC the code could provide for their own research projects.
- ❑ **6. Advanced school on Quantum Transport with SIESTA** will be organised by MAX (ICN2 node) in collaboration with Donostia International Physics Centre and will be held in San Sebastian (March 23-29, 2020) with the support of CECAM. The school will focus on the computation of electronic transport exploiting the non-equilibrium Green's function approach. The participants will learn the advanced features of SIESTA, such as the calculations of non-equilibrium properties using the TranSIESTA/TBtrans approach and the Python framework SISL. Recent advances in transport theory will be presented in the form of lectures and hands-on sessions on



hot topics in the field. The school will promote the interaction between participants and lecturers: the students will be asked to propose their actual case of study a month before the school and a session will be devoted to address them. The use of the NEGF technique for quantum transport in industry will be presented by Kurt Stokbro (Synopsis Inc.).

- ❑ **7. A Tutorial on AiiDA** will be organised by MAX (EPFL node) and will be held in Lithuania in spring-autumn 2020 with the collaboration of Vilnius University and Prof. Saulius Gražulis, and with the support of CECAM. The tutorial will see the participation of core AiiDA developers and will specific target attendance from Lithuania and its neighbouring countries (Latvia, Estonia, Belarus, Poland).
- ❑ **8. Advanced School on Materials and Molecular Modelling with Quantum ESPRESSO** organised by MAX (SISSA and ICTP nodes) at ICTP in Trieste (January 2021) with the support of QE foundation, ICTP and Psi-k. Based on a two-decade-long tradition of Quantum ESPRESSO training courses that have been held all over the world, the goal of the School is to enable participating scientists to combine the most advanced approaches to quantum materials simulation with an in-depth understanding of modern parallel architectures. The intensive program will offer theoretical and technical lectures, as well as demonstrations and dedicated hands-on sessions exploring HPC resources for scientific production. Participants will learn how to handle the research codes in the Quantum ESPRESSO more efficiently and how to exploit the several level of parallelism implemented. Hands-on sessions will be held on the SISSA-ICTP facility for high-end computing.
- ❑ **9. An advanced school on the CP2K code** is currently being planned in spring-summer 2020. The school, organized by MAX in collaboration with the CP2K developers team of the University of Zurich Lausanne, will probably be held at CECAM headquarter in Lausanne. The School will focus on advanced features of the code and the scaling of algorithms. Overview of background theory will be followed by hands-on sessions.
- ❑ **10. A one-day Blender course for scientific images in the materials domain** will be organized by MAX (CNR node) in Modena in June 2019. Blender is an open source 3D image creation suite, whose use can be tailored for domain-specific needs. The goal of the course is to provide hands-on knowledge for improving the quality of the



produced scientific images, of relevance for science as well as dissemination. The course is organized in response to a need expressed especially by MAX younger users.

### Specific Hackathons

In order to guarantee a proper training for the new generation of developers, the best format choice is the hackathon. For the organization and planning of such highly specific events, a special Committee has been established, formed by flagship code developers and HPC centres staff.

In particular, the already scheduled ones are:

- ❑ **11. AiiDA plugin migration workshop** was organised by MAX (EPFL node) in Lausanne (March 25-29, 2019). Developer oriented, the workshop had the aim of bearing the AiiDA software experts in the migration of their plugins to support both Python 2 and Python 3, as well as the changes introduced in AiiDA 1.0. URL:<http://www.aiida.net/aiida-plugins-migration-workshop-2019/>
- ❑ **12. Hackathon: exploring brand-new technology** will be organised by MAX (ICTP and CNR nodes) at ICTP in Trieste (fall 2019) with the support of MAX. As follow up of the successful event held at BSC in 2018 (URL: <http://www.max-centre.eu/max-hackathon/>) the event is meant to be an opportunity for meeting together several code developers from the MAX flagships code and technology experts from both HPC centres within MAX as well as from industry (i.e., third party software providers and computer vendors). The programme includes advanced training for developers on selected topics as well as coding activities targeting the development of either new features, performance improvements or performance portability to new architectures. The hackathon foresees the co-ordination by ARM, a MAX partner, with the main objective to allow flagship code developers to put the hands-on for porting kernels on ARM based platform. Other identified main topics are specific presentations on brand-new NVIDIA GPUs based platforms and technology along with the novelties introduced in OpenMP 5.0 which is expected to be standard *de facto* by then. The hackathon will be also the occasion to discuss together relevant improvement made with MAX2 to the flagships code, with particular focus on the technological aspects. Indeed, the motivation for this event is mostly by working groups in WP4 and WP1.
- ❑ **13. Hackathon: Development of common domain specific libraries** will be organised by MAX (SISSA, ICN2 and EPFL nodes) in Trieste at ICTP (November 25-29, 2019). This



event aims to gather all developers interested to develop interfaces to MAX libraries (URL: <http://www.max-centre.eu/libraries/>) and others into the MAX flagship codes. Other topics for this event are the quantum engines and generic activities of code gluing/refactoring. This hackathon will be crucial for the dissemination of MAX-WP1 outcomes. Hackathon attendees will learn how to realize architecture agnostic code, using WP1 libraries and general common APIs. A meeting aimed at best organizing the hackathon will be held this early summer in Bologna or Modena. WP1, WP2, WP3 and WP4 will jointly prepare common case studies for: the usage of the common APIs of the set of libraries - possibly giving priority to the high performance libraries: parallel linear algebra, FFT, convolvers and others; applications involving the common general API for quantum engines - these could involve WP5 developers as well, if Python interfaces will be available.

- ❑ **14. Hackathon: AiiDA plugins and workflows** will be organised by MAX (ICN2, EPFL and CINECA nodes) at CINECA or in Lausanne in the first half of 2020 (probably March-April) with the support of PRACE. The event aims at gathering code developers (either of MAX flagship codes or of other simulation codes) interested in developing new AiiDA plugins and workflows and at fostering interaction between AiiDA core developers and code owners. The participants will be indeed supported by a dedicated team of AiiDA developers and will work on the development of new AiiDA plugins (in particular for BigDFT, the MAX flagship code for which the AiiDA plugin is still missing), plugins for advanced features in SIESTA, and workflows for the different MAX flagship codes to support HPC performance.

### Training for trainers (developers of training materials)

- ❑ **15. Digital Learning for Electronic Structure Theory Codes:** A workshop will be organized by MAX (UGENT and EPFL nodes) in collaboration with CECAM and in Lausanne (CH) (January 2020). The aim of this workshop is to spread knowledge and lower thresholds to start using online teaching methods and creating educational resources to that end, with an emphasis on content that is relevant for MAX flagship codes. The approach will be practical and hands-on, and will provide the participants with a good overview of what they can do according to their background and the environment they operate in. In order to practice what we preach, lectures or code training sessions by eminent scientists from the electronic structure and HPC



community will be delivered at this workshop, and will be recorded, edited, elaborated upon and transformed into digital learning modules on the spot, by the participants. *Via* properly designed online training modules, MAX flagship codes can train their users in a more efficient way. The strongest advantage for all potential users (in particular those in industry) is that the availability of online training resources can lower the threshold to entry.

The timeline of the events organized by MaX until spring 2020 is shown below. An updated version of the training program will be reported in one year in the D8.2 deliverable.



Timeline of training events organized by MaX until July 2020.

### University course modules

In this section of the training plan, the academic environment is the target, with the Master and PhD students enrolled in the involved institutions. The planned training actions towards this audience include the following:

- MAX (EPFL team) contributed to with a module of 8 hours to the Doctoral School in Mathematics, Physics and Computer Science of the University of Udine (Italy), on bridging high-throughput simulations and web platform deployment. In particular, the course focused on explaining the scientific and technical challenges of HPC and HTC simulations, together with HPDA techniques. It then aimed attention on developing new web applets, focusing in particular on applications for education, using much of the technology that has been developed for the Materials Cloud and the AiiDA lab (see WP5). The course was designed with a multidisciplinary approach in mind, considering the multidisciplinary nature of the Doctoral School.



- MAX (ICTP and SISSA MAX nodes) will contribute for the next two years to modules of the joint SISSA/ICTP Master in High-Performance Computing (MHPC) (URL: <http://mhpc.it>). All the registered users to the MAX portal will be entitled to register for attending to modules of the MHPC under the essential requirement to have a minimum level of skill set in software development. Those modules range from the foundation of software development for scientific computing and parallel programming to advanced course for collaborative development, modularized design and software optimization. The curricula also include number of modules on advanced computational methodology in science and technology. The program of the MHPC will be linked to the MAX portable and visible to MAX registered users. From time to time, the coming soon modules of the MHPC will be especially advertised through the MAX network. It is expected that MAX partners will contribute to the master by proposing new modules, extending existing modules or giving seminars on computational materials science, advanced techniques for Exascale computing in material science and related topics.
- MAX (CNR team) will complement a University course on computational Physics at the University of Modena and Reggio Emilia with lectures on HPC and tutorials on computational materials science.
- Preparation of online courses and hands-on (see also event n. 15). Based on the past effort of the UGENT MAX node, an online course ([www.compmatphys.org](http://www.compmatphys.org)) on ab initio materials modeling is already available. The course is conceived using the QE package (MAX flagship code) and it is designed for an audience with a general science education, yet not having a specific background in theoretical physics (people in industry, experimental physicists, materials engineers, undergraduates or starting PhDs in physics or chemistry). The hands-on part of the course makes use of the Quantum Mobile VM. In the next period MAX will extend the course by including other MAX codes: Fleur and possibly Siesta that are already contained in the Quantum Mobile system, and also BigDFT for the future.

### Training through research in MAX laboratories

This part of the training actions will be coordinated MAX WP6, in particular the CNR and EPFL nodes. In the previous MAX phase, such instrument was demonstrated to be very powerful for both academic researchers (senior scientists and PhD students) and industrial researchers. HPC-Europa3 will support the academic users.

Since the beginning of MAX (December 2018), 16 visits have already occurred or scheduled.

### MAX contribution to EU transversal training initiatives

In the last months a strong collaborative effort was started in order to coordinate the domain specific training actions, organized by MAX in the field of materials, with activities



organized in neighbouring domains by other CoEs as well as cross-domain activities coordinated by FocusCoE or organized by PRACE. MAX is happy to offer and exchange training modules and materials, and to coordinate the calendars and promotion activities at all levels.

Throughout the course of CoE, MAX will be interacting with PRACE and FocusCoE, who established a dedicated CSA work package for this purpose.

Further needs and developments will probably emerge in the near future with the creation of Competence Centres, that will act as hubs offering interfaces between the needs of the national communities, including industrial and SME users, and the European ecosystem at large. MAX will work to offer its know-how and training expertise for activities that may be promoted by individual Competence Centres or by their network. At the time of this writing not enough details are known in order for MAX to make more specific plans in this direction, but we will be ready to include them in the next year.

## 5 Conclusions

The present document defines the plan of specialised training and education in computational materials science offered by MAX. MAX aims to offer training to both young code developers and academic and industrial users with the purpose of reaching a wide community at pan-European level. A number of training events among hands-on courses and hackathon is already scheduled for the first 18 months of MAX and the calendar will be constantly updated in the next few months. In addition to the aforementioned events, it has also been identified a plan for MAX contribution in academic course modules and MAX participation in EU transversal training initiatives. All the MAX training offers will follow a well defined strategy that finds its key points in (i) engaging industrial users, (ii) promoting the MAX activities at pan-European level, (iii) enlarging the pool of trained users of MAX flagship codes through on-line training materials, (iv) collecting the user needs and monitoring the impact of the training activities through common feedback surveys and (v) collecting accurate statistics of the participants to the events.

Importantly, MAX considers this plan is a living document that will be updated according to the evolution and needs of the materials research and the EuroHPC communities, in close coordination with the whole European HPC ecosystem.