



D8.2

First report on Training and Education

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Due date of deliverable: 31/05/2020
Actual submission date: 31/05/2020
Final version: 31/05/2020

Lead beneficiary: CNR (participant number 1)
Dissemination level: PU - Public



Document information

Project acronym:	MAX
Project full title:	Materials Design at the Exascale
Research Action Project type:	European Centre of Excellence in materials modelling, simulations and design
EC Grant agreement no.:	824143
Project starting / end date:	01/12/2018 (month 1) / 30/11/2021 (month 36)
Website:	www.max-centre.eu
Deliverable No.:	D8.2

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To be cited as: D. Varsano, M. Bartolacelli, M. C. Maschio et al., (2020): First report on Training and Education . Deliverable D8.2 of the H2020 project MAX (final version as of 31/05/2020). EC grant agreement no: 824143, CNR, Modena, Italy.

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D8.2 First report on Training and Education

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1 Executive Summary

Deliverable 8.2 reports on the education and training activities, including data on users participation and involvement. In [D8.1](#) we proposed our structured Training and Education plan, offering a domain-specific program at pan-European level and fostering a new generation of both developers and code users. Moreover, we described strategies and guidelines to reach a wide community also leveraging the collaboration with organizations such as CECAM, Psi-k and ICTP.

This plan is being effectively implemented through different actions, which in the first 18 months include:

- Organization of 6 schools (plus 2 already planned for the near future) dedicated to MAX flagship code users, with emphasis on their usage on pre-exascale machines. In all the schools, a relevant part of the training was in the form of hands-on sessions.
- Organization of 5 Hackathons and workshops (plus 2 already planned for the near future) devoted to the training of a new generation of code developers.
- MAX contributed to 4 Master programmes providing introductory courses to undergraduate students on computational materials science, hands-on sessions on usage of MAX flagship codes and best practice in their usage in HPC facilities.
- MAX hosted a large number of researchers in its labs providing both basic and specialized training on MAX codes and libraries.
- MAX actively contributed to schools and training events organized by other institutions.

These initiatives have resulted in the production of training material in form of tutorials and videolectures, that are published in a dedicated section of the MAX website and are available to the broader community.

Due to the COVID-19 outbreak, some of the events already planned had to be postponed. For some of them, MAX set up a revised online version of the schools. Moreover, MAX contributed to several online webinars to ensure its audience proper training during the lockdown. Due to the uncertainty of being able to organize events in presence in the future and also based on the experience acquired and the positive feedback received during the last months, MAX aims to extend its future online training offer. A strategy for MAX online training is also described in the present document.

The partners in charge of this WP are **CNR**, SISSA, ICN2, CEA, EPFL, Juelich, ICTP, UGE.



2 Introduction

In the first 18 months of activity, MAX CoE organized and planned a large set of education and training activities in computational materials science, with a focus on the flagship codes. The effort of MAX CoE is directed towards the training of both developers and users. The training activity focused on basic and advanced usage of the codes with an emphasis on best practice and efficient use of the codes in (pre-)exascale machines, libraries development and workflow implementations.

The strategy that MAX has defined in the [first deliverable D8.1](#) “Training and education programme” comprises different events structured as:

- **workshops, schools and hackathons:** in particular, hands-on workshops are meant to provide the technical know-how to both developers and users, schools in materials science to give state-of-the-art knowledge to the users, while hackathons and coding days/weeks bring together the advanced and the new developers;
- **teaching modules in University:** the targets are Master/PhD students and university teachers, on frontier computational methods within materials domain;
- **training through research:** one-on-one training by hosting academic and industrial researchers in CoE laboratories, for scientific projects involving the use of MAX flagship codes.

The partners involved in the present WP8 are CNR, SISSA, ICN2, CEA, EPFL, Juelich, ICTP, UGE, along with the collaboration with the CECAM and Psi-k organizations (supported through EPFL and Juelich, respectively). Furthermore, MAX gives relevance to every chance of coordination and contributions to transversal training initiatives (FocusCoE CSA, PRACE, other CoEs, HPC centers).

The first half of the activities planned in the MAX training program were organized along the plan and are reported below. The COVID-19 outbreak forced the rescheduling of some events that were already organized or in preparation and forced to severely and rapidly reconsider the methods of training delivery for these and future events. In this deliverable, we also describe the new strategies that will be implemented in the future in order to provide high quality training, preserving the standards exploiting online/virtual technologies (further description in paragraph 5).

Two out four of the activities expected in Spring 2020 did not take place (see Table 1, red color), since the pandemic affected their practical implementation: they will be rescheduled if there will be the conditions for a safe implementation; at the moment we cannot exclude the possibility to transform them in virtual events. Two other events, that are also postponed, were promptly re-organized in virtual edition (light blue in Table 1); they will also take place in presence if there will be the conditions. The events planned for the next Fall 2020 and Winter 2021 (orange color) are pending both in the date and in the format (in presence or online), as they are tied to the pandemic evolution and the safety rules that must be adopted in the future.



Training for MAX flagship codes users	
Fleur: hands-on school	2019-09-09/13
Quantum ESPRESSO: Summer School on Advanced Materials and Molecular Modelling	2019-09-16/20
Yambo: Computational School on Electronic Excitations in Novel Materials	2020-01-27/31
Siesta: Advanced School on Quantum Transport	POSTPONED 2020-03-23/27
Siesta: School on First-principles simulations of materials	POSTPONED 2020-05-04/8
AiiDA: School on High Throughput Computing	VIRTUAL EDITION 2020-07-07/10 IN PRESENCE - if possible 2021-07-07/10
Quantum ESPRESSO: Advanced School on Materials and Molecular Modelling	Winter 2021
MAX school on Computational Materials Science	TBD
Hackathons and workshops for code developers	
AiiDA plugin migration workshop	2019-03-25/29
Tutorial on writing reproducible workflows for computational materials science	2019-05-21/24
Hackathon: Development of common domain specific libraries	2019-11-25/29
Hackathon: AiiDA plugins and workflows	2020-02-17/21
ESL Workshop 2020	2020-02-17/28
Hackathon: exploring brand-new technology	Fall 2020
ESL Workshop 2021	Winter 2021
Visualisation and digital learning schools	
Visualisation - One day Blender course	2019-06-27
Digital Learning for Electronic Structure Theory Codes	1 DAY VIRTUAL EDITION 2020-04-28 IN PRESENCE - if possible Spring 2021

Table 1: MAX planned training activities. Postponed and future events are in red and orange respectively, while the one converted in virtual edition are in light blue.



3 Training events pre COVID-19

In the following, a description of the schools and workshops and the hackathons organized by MAX is presented following the separation depicted in Table 1, considering only the ones that took place in presence before the pandemic. The events are divided into different categories since they fulfil different tasks of WP8: following the definitions in the proposal, *i)* T8.1 task is devoted to filling the pipeline of new generation code developers and *ii)* T8.2 task is related to the Advanced training for academic and industrial code users. A further relevant activity in the MAX training is *iii)* T8.3 task, centered on the coordination and contributions to transversal training initiatives promoted by HPC centers and PRACE and events coordinated by the CSA.

3.1 Training for MAX flagship codes users

These events are devoted to the training of the users of MAX flagship codes through schools that provide basic and advanced knowledge on the first principles simulations in materials science.

1. Picking flowers: Hands-on FLEUR school
2. Summer School on Advanced Materials and Molecular Modelling with QUANTUM ESPRESSO
3. Computational School on Electronic Excitations in Novel Materials using the Yambo code

1. Picking flowers: Hands-on FLEUR

Venue and date: Forschungszentrum Jülich, Jülich (DE). September 9-13, 2019

Organizers: Forschungszentrum Jülich

Speakers: Marjana Lezaic, Gregor Michalicek, Christian-Roman Gerhorst, Daniel Wortmann, Gustav Bihlmayer, Jan-Philipp Hanke, Stefan Rost, Jens Bröder, Vasily Tseplyaev, Uliana Alekseeva, Matthias Redies, Christoph Friedrich, Irene Aguilera, Yuriy Mokrousov, Markus Hoffmann

Topics: this tutorial focused on training the participants in using the all-electron FLAPW DFT code FLEUR and associated codes like Spex-FLEUR, a code for many-body perturbation theory, and G-FLEUR, an embedding code. In addition to similar previous tutorials it also addressed the usage of FLEUR within the AiiDA infrastructure to build automatic workflows applicable to materials screening applications. The tutorial covered theoretical lectures to provide the necessary methodological and physical background to professionally use the FLEUR code family and enabled the participants to



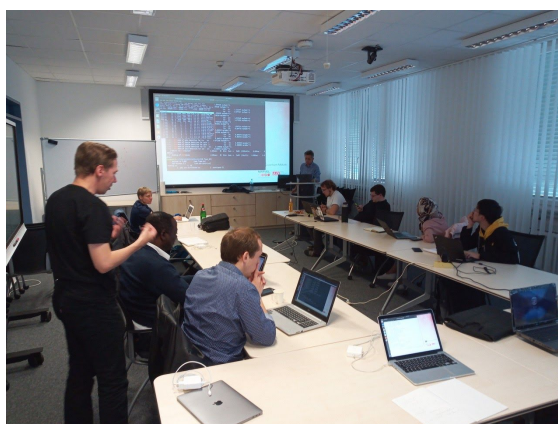
benefit from the strengths of the codes. Hands-on sessions were provided to get in touch with the codes from a practical perspective. The Hands-on session made use of the [Quantum Mobile](#) virtual machine. Video lectures were recorded and are collected in the [training section](#) of the MAX website.

Type of event: T8.2 - Advanced training for academic and industrial code users

N of participants: 10

Overall assessment: The feedback received from the participants has been extremely positive, and few suggestions from the participants help in further improving. Overall score from anonymous feedback questionnaire 5.0/5

Website: <https://www.cecarn.org/workshop-details/136>



2. Summer School on Advanced Materials and Molecular Modelling with Quantum ESPRESSO

Venue and date: JSI, Ljubljana (SLO). September 16-20, 2019

Organizers: QE foundation, MAX, Jožef Stefan Institute, CECAM

Speakers: Stefano Baroni (SISSA, Trieste), Anton Kokalj (Jožef Stefan Institute, Ljubljana), Paolo Giannozzi (DMIF, Udine), Pietro Delugas (SISSA, Trieste), Iurii Timrov (EPLF, Lausanne), Giovanni Pizzi (EPLF, Lausanne), Carlo Cavazzoni (CINECA, Bologna), Pietro Bonfà (Università degli Studi di Parma, Parma), Željko Šljivančanin (Institute of Nuclear Sciences, Vinča), Dino Novko (Institute of Physics, Zagreb)

Topics: The aim of the school was to introduce students, postdocs, and other researchers to materials and molecular modelling with Quantum ESPRESSO. The school covered basic concepts as well as recent advances and developments, with emphasis on density-functional-theory based methods and high-performance computing. The school included both theoretical and practical hands-on sessions, involving the use of a virtual machine based on the [Quantum Mobile](#).



Type of event: T8.2 - Advanced training for academic and industrial code users

N of participants: 59

Overall assessment: The participants highly appreciated the organization of the school, and the hands-on sessions were extremely fruitful. The use of the Quantum Mobile virtual machine was also positively evaluated. Overall score from the anonymous feedback questionnaires 5.0/5.

Website: <http://qe2019.ijs.si/>



3. Computational School on Electronic Excitations in Novel Materials using the Yambo code

Venue and date: ICTP Trieste (IT). January 27-31, 2020

Organizers: MAX, Psi-k

Speakers: Seyedeh Samaneh Ataei (CNR-NANO, Italy), Claudio Attaccalite (CNRS, CINAM, Aix-Marseille Université, France), Stefano Baroni (SISSA, Italy), Miki Bonacci (University of Modena and Reggio Emilia, Italy), Andrea Ferretti (CNR-NANO, Italy), Andrea Marini (CNR-ISM, Italy), Pedro Melo (University of Liege, Belgium), Alejandro Molina-Sanchez (IINL, Portugal), Paolo Moras (CNR-ISM, Italy), Fulvio Paleari (CNR-ISM, Italy), Maurizia Palummo (University of Rome "Tor Vergata", Italy), Davide Sangalli (CNR-ISM, Italy), Michiel Jan Van Setten (IMEC, Belgium), Daniele Varsano (CNR-NANO, Italy), Ludger Wirtz (Université du Luxembourg, Luxembourg)

Topics: The school introduced participants to post-DFT simulations, in particular many-body perturbation theory (MBPT) approaches and provided training in the calculation of electronic and optical properties of materials. The school included both theoretical and practical hands-on sessions using the Yambo code, along with the use of [Quantum Mobile](#). Sessions were dedicated to the code usage in HPC facilities and user



focus groups sessions were also organized where students could address specific questions regarding the code usage in the context of their own research.

Type of event: T8.2 - Advanced training for academic and industrial code users

N of participants: 56

Overall assessment: The school raised high interest in the community, as more than 250 applications were sent. Because of that, video lectures were uploaded day by day in the channel dedicated to the school and are now collected in the [training section](#) of the MAX website. The user focus session was highly appreciated. Overall score from anonymous feedback questionnaire 5.0/5

Website: <http://indico.ictp.it/event/9018/>



3.2 Hackathons and workshops for code developers

Beside the classical workshops, in order to guarantee a proper training for the new generations of *developers*, the format of choice is the hackathon since it allows learning by doing and close contact with leading code developers and experts. 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.

1. AiiDA plugin migration workshop
2. Tutorial on writing reproducible workflows for computational materials science
3. Hackathon: Development of common domain specific libraries
4. Hackathon: AiiDA plugins and workflows
5. ESL Workshop 2020



1. AiiDA plugin migration workshop

Venue and date: EPFL - Lausanne (CH). March 25-29, 2019

Organizers: MARVEL, MAX

Speakers: Sebastiaan P. Huber (EPFL), Oscar Arbelaez (EPFL), Leopold Talirz (EPFL), Giovanni Pizzi (EPFL)

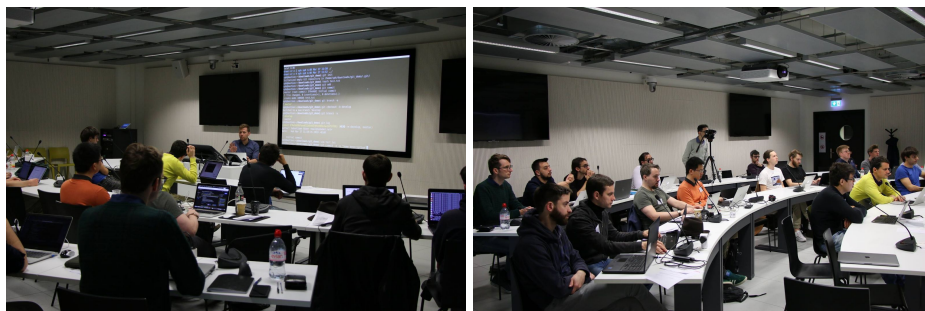
Topics: The aim of this workshop was to directly support AiiDA plugin developers in the migration of the existing plugins to support both python 2 and python 3, as well as the changes introduced in AiiDA 1.0. Some sessions were devoted to discussions on plugin interfaces and their homogenisation and common APIs, exploiting this unique occasion bringing together many plugin developers. The lectures were recorded and uploaded [online](#).

Type of event: T8.1 - Filling the pipeline of new generation code developers

N of participants: 25

Overall assessment: The workshop was extremely impactful in migrating the majority of available AiiDA plugins to the most recent version of the code, and to explain and implement modern code development practices (testing, continuous integration, python2+3 support, ...) in all of them. The feedback from the participants was extremely positive both from the point of view of the support they received from the AiiDA development team, and on the impact of the workshop on their codes. Also the organisers felt that the event was a success, and that it helped strengthen the feeling of an AiiDA plugin-ecosystem community. Overall score from anonymous feedback questionnaire 4.5/5.

Website: <http://www.aiida.net/aiida-plugins-migration-workshop-2019/>



2. Tutorial on writing reproducible workflows for computational materials science

Venue and date: EPFL, Lausanne (CH). May 21-24, 2019

Organizers: MAX, MARVEL, Psi-k, Swissuniversities, Intersect, EPFL



Speakers: Stefaan Cottenier (UGent, BE), Marco Govoni (ANL, US), Fawzi Mohamed (FHI, GE), Guido Petretto (UC Louvain, BE)

Topics: this tutorial was designed to get Master students, PhD students and Postdocs from the field of computational materials science started with writing reproducible workflows. Participants will be introduced to the state of the art in workflow management and high-throughput computations by experts in the field, and gain in-depth hands-on experience using a tool that they can directly apply to their own research.

Type of event: T8.2 - Advanced training for academic and industrial code users

N of participants: 55

Overall assessment: the feedback of the tutorial has been highly positive, and the users were very satisfied with the hands on organization and the available materials. Overall score from anonymous feedback questionnaire was 4.0/5

Website: <http://www.aiida.net/news/tutorial-writing-reproducible-workflows/>



3. Hackathon: development of common domain specific libraries

Venue and date: ICTP Trieste (IT). November 25-29, 2019

Organizers: MAX

Speakers: Dr. Pietro Bonfà - University of Parma and CNR-Nano; Dr. Geoff Womeldorff - LANL

Topics: The hackathon meeting was meant to update the MAX community of developers to the state of the art implementations and future road-maps of the MAX libraries. At the same time it was an opportunity for young scientists to meet the MAX developer while working together for interfacing MAX libraries to their code. The program was structured with a mix of direct presentations and a number of hacking sessions.

Type of event: T8.1 - Filling the pipeline of new generation code developers



N of participants: 24

Overall assessment: Feedback from the participants unanimously indicated a positive experience of both exchange between the participants and to converge ongoing branches of development within MAX.

Website: <http://indico.ictp.it/event/9172/overview>



4. AiiDA Hackathon: developing code plugins and robust scientific workflows

Venue and date: CINECA, Bologna (IT). February 17-21, 2020

Organizer: MARVEL, MAX, PRACE

Speakers: Sebastiaan Huber (EPFL), Aliaksandr Yakutovich (EPFL), Luigi Genovese (CEA), Giovanni Pizzi (EPFL), Leopold Talirz (EPFL)

Topics: In this Hackathon AiiDA plugin developers showed best practices and useful tips on: code development practices (automated testing, continuous integration, code style checks, packaging, distribution...); writing reusable, robust and modular workflows; taking full advantage of the AiiDA v1.0 API. In addition, during the event common APIs for workflows for the computation of certain materials properties were discussed and defined. When adopted by plugin developers, these common APIs enable AiiDA users to compute a materials property using different codes without the need to know the interface of each plugin in detail.

Type of event: T8.1 - Filling the pipeline of new generation code developers; T8.3 Coordination and contributions to transversal training initiatives

N of participants: 21

Overall assessment: The working group gathered new interesting ideas and traced a route on the development of the framework. In particular, the code plugins had a wide improvement in their development thanks to the organizers' help. Finally, the

containerization strategies and how plugin development can contribute to Materials Cloud were fruitfully discussed.

Website: <http://www.aiida.net/news/aiida-hackathon-developing-code-plugins-and-robot-scientific-workflows-cineca-bologna-italy/>



5. Integration of ESL modules into electronic-structure codes

Venue and date: EPFL, Lausanne (CH). February 17-28, 2020

Organizers: ESL, CECAM, e-CAM, MAX, Psi-k

Speakers: Nick R. Papior (Technical University of Denmark), Damien Caliste (CEA), Martin Lueders (Max Planck Institute), Alan O'Cais (Jülich Supercomputing Centre), Stefano de Gironcoli (SISSA), Arash Mostofi (Imperial College London), Volker Blum (Duke University), Paul Saxe (MolSSI)

Topics: the Electronic Structure Library (ESL) community organizes workshops that aim at the development and maintenance of libraries [esl, esl-gitlab] as well as the modification of existing codes to benefit from libraries by adopting their use. This edition (2 days general discussion and 2 weeks of coding) was devoted to demonstrating ESL capabilities by building an electronic structure code from scratch using components present within ESL.

Type of event: T8.2 - Advanced training for academic and industrial code users

N of participants: 17

MAX members: Stefano de Gironcoli and Alberto Garcia, both involved in planning the coding work. SdG as speaker describing the work done to disentangle the Kohn-Sham



Solvers used in Quantum ESPRESSO; AG as speaker in the general discussion phase describing the libgridxc and libpsml libraries,

Overall assessment: the workshop had a very active participation from a small group of coders: two codes, one employing an atomic orbital basis set and one using plane-waves, were built from scratch making use of the libraries present in the ESL bundle. Participants reported general satisfaction in an on-line distributed questionnaire.

Website: <https://www.cecim.org/workshop-details/85/>



3.3 Visualization and digital learning schools

Besides schools focused on flagship codes and hackathons that are at the core of the MAX training, a few events dedicated to complementary aspects have been organized. Here we report two examples: i) a course dedicated to professional creation of scientific images using the open-source 3D computer graphics suite Blender, with the aim to improve the ability in disseminating scientific results in an attractive way; ii) a course on how to realize an effective and proper digital training in computational electronic structure theory codes. The latter event gathered experts in digital training and provided useful insight to define best tools for the online training on MAX flagship codes, which turned out to be of great importance in light of the organization of future post COVID-19 MAX training.

1. One day Blender course - for scientific images

Venue and date: CNR Nano, Modena (IT). June 27, 2019

Organizers: MAX, TAME plasmons, Intersect, Q-sort

Speakers: Paul Melis and Casper van Leeuwen - SURFsara Amsterdam

Topics: the course on Blender aims to improve the quality of scientific communication and will provide hands-on knowledge of producing great images and animations from 3D (scientific) data with a focus on Materials science.

Type of event: T8.2 - Advanced training for academic and industrial code users



N of participants: 26

Overall assessment The course has been appreciated by the attendants: the objectives and the exercise were clear, even though the difficulty in using the software could have required more sessions of work. Overall score from anonymous feedback questionnaire 4.0/5

Website: <http://www.max-centre.eu/events/one-day-blender-course-modena-it>



2. Digital learning for Electronic Structure Theory codes

Initially scheduled for April 27-30, a one-day online event titled “[Digital Learning after its Black Swan](#)” was organized on April 28th because of COVID-19 pandemic. All the details can be found in paragraph 4.

3.4 Participants statistics and considerations for future activities

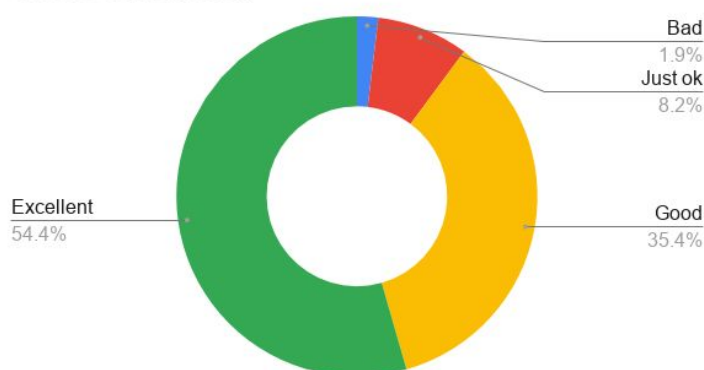
In order to provide a measurable impact of the training activities, MAX collected for each event detailed statistics about provenance and gender of the participants and the satisfaction of the attendees is measured through an anonymous feedback form. In the following, the overall statistics of the activities that took place before COVID-19 outbreak is reported.

The total of 9 events (schools, tutorials, hackathons) counted so far a total of approximately 300 participants.

The metrics for assessing the quality of the training activities covers the range *1=very poor, 2=bad, 3=just ok, 4=good, 5=excellent*. The overall user satisfaction, based on the 9 surveys for each school, reached a very positive evaluation of 4.7/5.

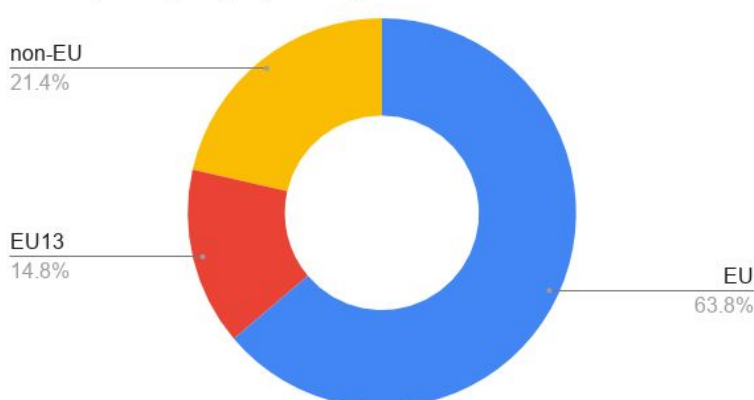


User's satisfaction



Overall, 14.8% of participants came from the countries of the EU13 area and 21.4% came from outside Europe. The remaining 63.8% came from European countries.

Participant geographical provenance

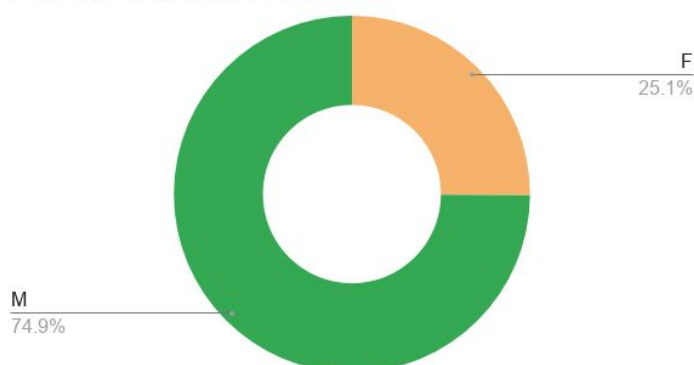


To enlarge the pan-European participation in training initiatives, MAX included in the training plan 3 events to be delivered in Eastern Europe. These events involve local experts both in the organization and in the team of lecturers. In the summer school on Advanced Materials and Molecular Modeling held in Ljubljana (Slovenia) in September 2019, more than 55% of the participants came from EU13 countries. Two additional events in countries outside the consortium were initially planned: a school on First-principles simulations of materials with SIESTA to be held in Prague (CZ) in May 2020 and an AiiDA tutorial in Vilnius (LT) Summer 2020. As mentioned above, these events will be rescheduled because of the COVID-19 pandemic.

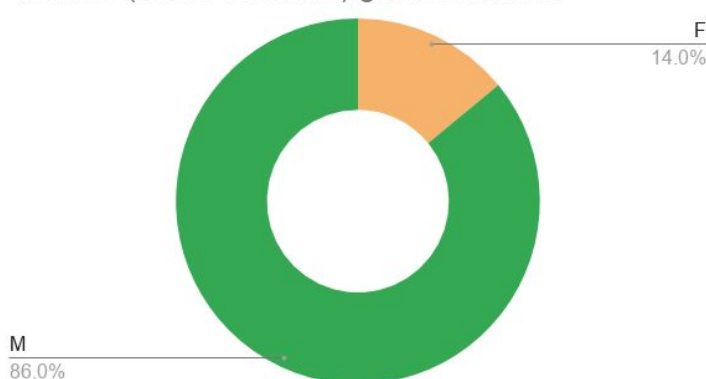
Within the pool of participants, 25.1% of the total were women, while the percentage of women that delivered the training (hands-on sessions tutors and lecturers) was 14.0% .



Participant gender balance



Trainers (tutors+lecturers) gender balance



MAX is well aware and concerned of the gender imbalance that is still present and is seriously addressing the problem. The actions that MAX has already put in place to solve this issue include:

- Particular care taken in the phase of the selection of the applicants to ensure participation of the maximum number of women: as an example, 40% of the full fellowships available for the 'Computational school on electronic excitations in novel materials' (Trieste, January 2020) were awarded to women.
- Further applications from women candidates to be promoted through different channels including networks of young women as well as women professors who may encourage their attendance. Dedicated promotion through our social media (women are 42% of the audience).
- MAX has promoted and will co-sponsor a women networking session within the major community event planned next year, the [Psi-K 2020 Conference](#) (Lausanne, officially postponed to August 2021), with over 1000 participants expected. The Program Committee has already approved the proposal, which will be designed to allow for direct interactions among senior participants and students. This will be expected to be a special opportunity to engage young women in MAX activities and training.



- MAX is working to increase the number of women involved in the organization of the events and among the invited lecturers. This is a condition for the dissemination events supported by MAX within the Cecam and Psi-k workshop and event programs.

To conclude the overview of the statistics, attendees to MAX schools and workshops came mostly from academia registering only 2.2% of industrial users. Experience and statistics has shown that industrial users are not attracted by the school format. However, other routes have been followed to set successful training towards industrial users.

Starting from the High Level Consulting services that MAX offers, industry often requests “face-to-face” training for its employees, and this becomes a key part of subsequent contracts. In particular, ICN2 MaX partner started a collaboration with an ISV interested in the use of the Siesta flagship code for the study of topological insulators (10 person days already delivered, the remaining 80 person-days by the end of 2021). Furthermore, the same partner delivered 5 person-days of training on the NEB (nudged elastic band) method and 2 person-days of training on the use of a GUI interface for SIESTA code.

EPFL MAX partner delivered training to industrial users regarding the use of the AiiDA platform for glass manufacturers (2 person-days) and the set up of the AiiDA lab for R&D lithium-ion batteries industry (5 person-days).

Finally MAX (CNR and CINECA) started to provide training and support to the Air Liquide company for a total of 40 person-days. The training activity involves both the installation and configuration of the AiiDA framework targeted at the private cluster and specific environment needed by the industrial company and a training focused on the usage of the platform in combination with other MAX flagship codes. However, due to the COVID-19 issue, it was not possible to proceed with a targeted installation and it will be delivered as soon as possible following the evolution of the COVID-19 outbreak.

3.5 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.

In particular, during the first 18 months, MAX participated in several activities proposed by FocusCoE. The awareness that HPC training plays an important role in sustaining a pool of researchers and developers - who can exploit the full potential of supercomputers - has driven all the CoEs in outlining plenty of initiatives, and in particular in adhering to the concerted ones proposed by FocusCoE.

On October 8th, 2019, MAX contributed in the European HPC Training Stakeholder Workshop in Brussels, in which the European CoEs gathered both to define what are the



training requirements from different domains/target audiences, and to examine how these requirements may be met by existing or new European and national programmes on HPC training.

On April 28th, 2020, the second European HPC Training Stakeholder Workshop took place as a meeting online because of the COVID-19 pandemic. During the briefing, FocusCoE presented a tool called “Training Registry” deployed to collect training events information from different projects/centres in order to facilitate a pan-European view of available HPC training services/offerings. MAX promptly joined the portal uploading the existing MAX training offers and will update the Registry with the upcoming events.

Most of the training events were organized in collaboration with community organizations as CECAM (3 events), Psi-K (3 events) and ICTP (2 events), among others. Some of the events were also organized in synergy with other CoE and EU initiatives as PRACE. All postponed events already planned are in collaboration with CECAM (3 events) while the future ones in 2021 will have co-funded resources with ICTP and Psi-k.

3.6 Participation of MAX members as lecturers in other schools

The training strategy of MAX also includes contributions to schools and training events organized outside the CoE. In these events the training focused on MAX flagship codes including hands-on and best practice in the code usage in pre-exascale machines. The lectures offered by MAX members are listed below:



- 1st Central African School on Electronic Structure Methods and Applications (CASESMA) November 18-23, 2019 Dschang, Cameroon. School supported by ICTP.

MAX member: Andrea Marini (CNR), Nicola Marzari and Giovanni Pizzi (both EPFL - overseeing and preparation of materials for lessons)

MAX Codes: Yambo and Quantum ESPRESSO

Number of participants: 88

The scientific program focused on ab initio molecular dynamics and many body perturbation theory with a brief introduction on Quantum ESPRESSO and a wide use of Yambo code. All the tutorials, exercises and simulations were run on the Quantum Mobile.

- [Eastern Africa School on Electronic Structure Methods and Applications - Addis Ababa](#)

Period: July 1-5, 2019

MaX members: Nicola Marzari and Giovanni Pizzi (both EPFL - overseeing and preparation of materials for lessons)

Number of participants: 52

The workshop covered the fundamentals and hands-on training on advanced and widely used computational methods (i.e., Density Functional Theory, Molecular Dynamics and Monte Carlo methods), reviewing recent scientific advances in the field of emerging electrochemical energy conversion and storage technologies such as advanced rechargeable batteries, supercapacitors, fuel cells and solar cells. The main goal of this scientific conference is to help junior researchers in some Universities of Ethiopia, who are interested to work on various computational methods for studying materials properties (i.e., electronic, optical and magnetic). This course featured the use of Quantum ESPRESSO and a tailored version of the [Quantum Mobile](#) virtual machine.

- [1st TUMIEE Training School in Rethymno, Crete \(Greece\)](#) 23/09 - 4/10 2019, Rethymno Crete (Greece): "Training young researchers on multidisciplinary approaches to electronic excitation problems". A 10 days school supported by TUMIEE Cost Action.

MAX member: Davide Sangalli (CNR)

MAX Codes: Yambo and Quantum ESPRESSO

*Number of participants: 30*

The goal of this training school was to transmit the state-of-the-art in the field of electronic excitation to young researchers, preferably, PhD students already involved in research activities in the field.

- [High Performance Computing – ELCOREL workshop, Altafulla, Tarragona \(Spain\) in June 3-5th, 2019](#)

MAX member: Miguel Pruneda (ICN2)

MAX Codes: Siesta

Number of participants: 22

The “High Performance Computing” ELCOREL workshop will be held in Altafulla, Tarragona (Spain) on June 3 – 5th, 2019, as part of the ELCOREL meeting. The aim of ELCOREL is to train young researchers in all scientific and technological aspects of the storage of renewable electricity into fuels and chemicals. MP holds a lesson and an hands-on session on MD Transport Siesta.

- [MSSC2019 - Ab initio Modelling in Solid State Chemistry](#), London (UK), 16/09 - 20/09/2019. School supported by Psi-K and Thomas Young Center

MAX member: Andrea Ferretti (CNR)

MAX Codes: Quantum ESPRESSO, Yambo

Number of participants: 25

The school provided an overview of the possibilities offered by ab initio quantum mechanical techniques as adopted by the CRYSTAL code when applied to the characterization of crystalline materials. A particular emphasis was given to practical issues in obtaining reliable data efficiently using modern computer hardware. MAX contribution consisted in lecturing on the theoretical foundations of the Landauer theory for coherent transport through nanjunctions, discussing its implementation in ab initio computational codes, and presenting some recent scientific results obtained through this machinery. Reference to MaX codes Quantum ESPRESSO and Yambo and to scientific results obtained from them was made during the lecture.



- [VASP and AiiDA workshop at SINTEF, September 23-27, 2019 - Oslo \(Norway\)](#)

MAX member: Sebastian Huber (EPFL)

MAX Codes: AiiDA - Quantum Mobile

Number of participants: 45

Alongside the VASP tutorials, an introduction to AiiDA was given in order to establish the importance of data provenance, sharing and elevated efficiencies offered. Finally, a tutorial on the AiiDA-VASP plugin for AiiDA was given, which is suitable for more advanced VASP users seeking to increase productivity and usability.

- [CODES@OEHI Hackathon 2019](#), October 28-29, 2019 - CINECA Casalecchio di Reno (Italy)

MAX member: Daniele Cesarini (Cineca), Fabrizio Magugliani (E4), Arm

Number of participants: 12

The goal of this 2-day hands-on workshop was for current or prospective users of Arm-based HPC systems to port their applications to such systems or to further optimize already ported applications. Expert introduction into current Arm-based hardware architectures and the Arm development ecosystem was provided.

- [School on Wannier90v3.0: new features and applications](#), 25-27th March 2020 – Virtual Edition

MAX member: Giovanni Pizzi (EPFL)

MAX Codes: AiiDA, Quantum Mobile

Number of participants: 40

The 3-day school focused on the state-of-the-art functionalities of the Wannier90 code, with a particular focus on the latest developments (topological, transport and optical properties; automated Wannier functions; high throughput calculations) to both new and experienced users, and developers alike. The hands-on tutorials made use of the Quantum mobile and the AiiDA automated wannierisation workflow was presented.



3.7 Teaching modules in University

In the MAX training plan, a significant part is given by courses and seminars provided to undergraduate Master students and PhD students as well as University teachers, who wish to learn the use of frontier computational methods within their domain. In order to do so, several commitments were taken and have been realized by MAX partners.

- [Hands-on course "Computational Laboratory of Quantum Mechanics"](#)

University of Modena and Reggio Emilia, UNIMORE, Italy

Period: 23/10/2019 - 17/12/2019

MAX members: Andrea Ferretti (CNR) and Daniele Varsano (CNR)

Number of participants: 10

The hands-on module held by A. Ferretti (CNR) and D. Varsano (CNR) was part of the Laboratory of Computational Quantum Mechanics held by Alice Ruini in the Master programme in the University of Modena and Reggio Emilia. Within this course, the students were introduced to the usage of the MAX flagship code Quantum ESPRESSO for the calculations of fundamental quantities related to energetics and electronic structure of bulk, surface and molecular systems. At the end of the course, the students developed the capability to independently set up simulations for simple crystal structures, by adopting the better-suited configurations for the different situations, developed the ability to independently evaluate the solution strategies of new (i.e. not treated in the course) physical problems. The students also developed the ability to report on the results of numerical simulations of material properties, by using a suitable specialized language. Furthermore, at the beginning of the course the students acquired also knowledge of basic Unix language and scripting and developed the ability to analyze physical problems that one can encounter also in non-physical disciplinary areas and to set up appropriate solution strategies. At the end of the course, students also acquired knowledge on parallelization strategies of the used code and learned about best practice in running calculations in parallel machines and HPC infrastructure.

- [SISSA/ICTP Master in HPC \(MHPC\)](#)

Period: a.y. 2019/2020

MAX members: Stefano De Gironcoli (SISSA), Ivan Girotto and Ralph Gebauer (ICTP)

Number of participants: 16

The joint SISSA/ICTP Master in HPC (MHPC) is a successful professional program at its 7th edition. It is aimed to train a mix class of at most 15 students (closed number,



few exceptions allowed) per year from M.Sc graduated, to post-docs and PhDs, providing the technological background needed to master modern HPC applications. A first part of the program is dedicated to HPC technology, a second part to the main computational problems on both HPC, AI and machine learning, followed by a 6 months of thesis on a practical project. At the moment the MHPC registers 100% employment of the former students, easily finding job positions in either industry, public research or academia. MAX members Stefano De Gironcoli (SISSA), Ivan Girotto and Ralph Gebauer (ICTP) are lecturers of the program as well as members of the Scientific Council of the (MHPC). In particular, Ivan Girotto is responsible for the course of "Parallel Programming for HPC", teaching main parallel programming paradigms such as shared and distributed memory along with CUDA; Ralph Gebauer is responsible for the course of "Parallel FFT" mainly teaching how to parallelize a distributed 3D FFT; while Stefano De Gironcoli is responsible for the course on "Basics of Electronic Structure, from blackboard to source code".

- [Contribution in the RWTH Aachen University Master Programme.](#)

Period: winter semester 2019/2020

MAX members: Stefan Blügel (Jülich) and Gregor Michalicek (Jülich)

Number of participants: 7

MAX contributed to the RWTH Aachen University Master Programme with a series of lectures and hands-on tutorial in electronic structure calculations. The theoretical lectures introduced the students to the foundations of density functional theory and to relevant approximations in ab-initio methods for electronic structure calculations. Different extensions on DFT were discussed, e.g., many-body perturbation theory (MBPT) in the GW approximation of Hedin. The exercise to the lecture had the form of a hands-on tutorial on the MAX flagship code Fleur. Beyond teaching the basics of the full-potential linearized augmented planewave (FLAPW) method the tutorial covered the calculation of, e.g., lattice constants, lattice structures, surface properties like surface energy and work functions, density of states and band structures of solids, local magnetic moments, magnetic exchange interactions and magnetic anisotropy, non-collinear magnetic structures such as spin spirals. The GW approximation to MBPT was covered by introducing the students to the Fleur SPEX code.



- Course on [Atomistic and Quantum Simulation of Materials](#) at EPFL

Period: spring semester 2019/2020

MAX members: Nicola Marzari (EPFL), Francisco Ramirez as teaching assistant (EPFL).

Number of participants: 25

University course at EPFL for Master/PhD students that covers basic topics of materials simulations. This includes both classical and quantum models: electronic-structure and first-principles approaches, temperature and thermodynamic averages, Monte Carlo sampling and molecular dynamics simulations. It also deals with how to obtain materials' properties from simulations: mechanical properties, band structures and electrical transport, molecular dynamics and diffusion coefficients, and phonons and vibrational spectroscopies. The course consists of 32 total hours of lectures and 24 total hours of computational labs practical work. This course featured the use of Quantum ESPRESSO and the QuantumMobile virtual machine.

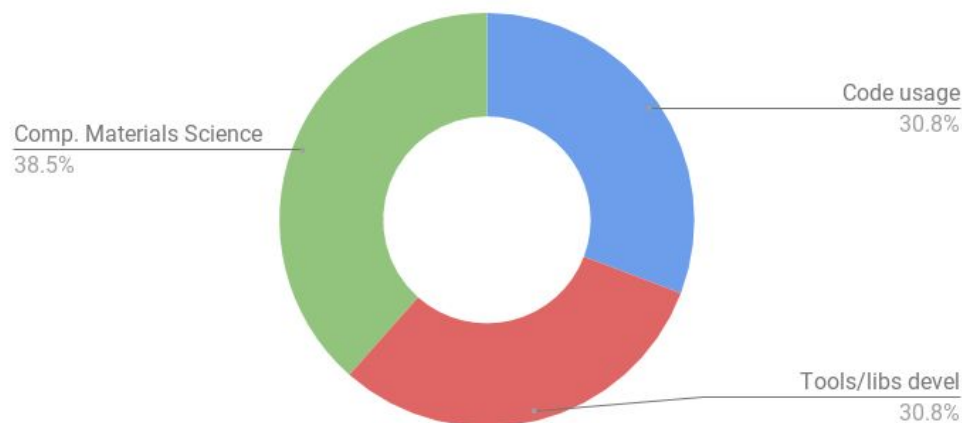
3.8 Training through research

As experienced in MAX 2015-2018, another successful channel of training is provided directly by hosting researchers in the CoE labs. Such an instrument is very powerful as it can reach both industrial researchers and academic researchers/PhD students. In these first 18 months, overall 38 young researchers were hosted in MAX Labs.

The aim is introducing students and young researchers in the functionalities of the MAX flagship codes and in the method/theory implemented therein for applications in the field of tribology, electronic, optical and transport properties of the material, high-throughput computation and high-throughput data analysis.



Training in CoE labs



Overall, the training visits organized in the CoE labs can be classified among different purposes: a basic training on flagship code usage (Code Usage) and an advanced training on flagship code related to a research project in computational materials science (Computational Materials Science), after which the visitors were able to set up specific calculations autonomously. Finally, a training devoted to developing tools and libraries (Tools/libs devel.) for the flagship code, in order to implement new features in the codes for specific scientific needs. The full list of researchers visiting MAX labs, host institutions and purpose of the visit can be found in Appendix 2. In this training activity MAX has benefited from the synergy with the HPC-Europa3 programme. Unfortunately some planned visits to MAX labs have been postponed because of the COVID-19 outbreak and have been rescheduled.

4 Online training activities

As anticipated above, the COVID-19 outbreak forced plenty of variations in training activities organized by MAX and its partners. In this section we report the online training activities that MAX has organized in the last two months to ensure its audience a proper training during the lockdown. Furthermore we sketch a strategy MAX plans to adopt to continue to deliver online training. This procedure will be also accompanied by in-person events that will be organized as soon as there are opportunities to be able to carry them out safely:

- As mentioned in the introduction (see Table 1), the MAX event "[Digital Learning for Electronic Structure Theory Codes](#)", scheduled for April 27-30 in collaboration with CECAM, was postponed to a future date. Nevertheless, a one-day online event titled "[Digital Learning after its Black Swan](#)" (video and materials available in the event page), was promptly organized on April 28th. The goal of the workshop, in its original version, was to "train the trainer" in delivering a proper training - especially in the field of Electronic Structure Theory Codes - through digital tools. Now more than



ever, such an event was a very useful time of reflection in order to define the best tools for the online training. In this meeting several scientists --mostly from the electronic structure theory community-- shared experiences and brainstormed about the future of learning and training. All contributions were recorded and are available online. To facilitate the consultation of the materials, the participants collaboratively wrote a summary of each talk during the event, which was afterwards reviewed by the corresponding speaker. These written summaries are shipped with the video of each talk. During the Q&A session, participants submitted their questions in written form. The speakers answered orally as the questions came in, and most speakers provided later a written version of their answers as well. All the reflections and brainstorming exercises were written and uploaded online as well. Several participants wrote a one-paragraph take-away message, and these are collected in one summarizing document as general and positive feedback.

The overall conclusion from this event was that there are surprisingly many flavours of online learning and online conferences, and for many situations there will be a flavour that fits. No-one knows all of them, exchange of ideas and inspiring each other is very important. Some of the methods/formats that have been tried within this workshop will inspire others, and the result of the brainstorming exercises was considered to be very useful and enlightening.

Organizers: UGE, MAX, CECAM

Speakers: Stefaan Cottenier (Ghent University), Gian-Marco Rignanese (Université catholique de Louvain), Francesco Sottile (Ecole Polytechnique), Eric Vantroyen (Ecole Polytechnique), Jörn Loviscach (FH Bielefeld University of Applied Sciences), Brian Mulligan (Institute of Technology Sligo), Giovanni Pizzi (EPFL), Gareth Tribello (Queen's University Belfast)

Number of participants: 19

- **MAX webinars series on flagship codes:**

MAX organised a webinar series presenting the latest developments of its flagship codes and their usage. Importantly, the focus is on the perspective of use and performance of MAX codes on heterogeneous architectures, in view of the forthcoming EuroHPC machines.

The first appointments were held during the month of May 2020.

- ❑ The first [webinar](#) was dedicated to the Quantum ESPRESSO code usage in new GPU based HPC systems and took place on 13/05/2020.



The main topics discussed during the webinar were:

- Status and features of Quantum ESPRESSO running on GPU-based systems
- How to use Quantum ESPRESSO optimally on heterogeneous HPC systems
- How to compile and tune up Quantum ESPRESSO for GPUs, and which tools and libraries are needed.

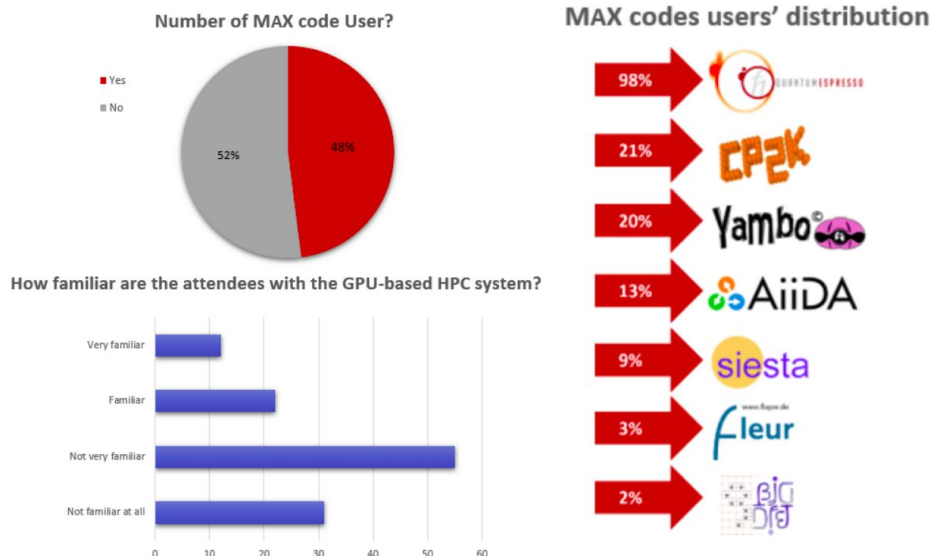
Speakers: Pietro Delugas (SISSA), Fabio Affinito (CINECA), Pietro Bonfà (University of Parma, CNR)

Attendance: **193 active participants** at the peak, the quality of the participants we noted were high profiled and fully aligned with the context of the Webinar. The audience never went below the threshold of 160 persons throughout the whole event. The average engagement degree was high too.

Registered people: 270 people, with a low no show rate of 30%.

Interactions: besides a continuous flow of comments in the chat, **67 questions** were posed to the speakers.

Poll Questions: during the webinar we set **3 Polls** (short & immediate surveys). These are the results coming out of 132 respondents:



Training materials: both the slides and Webinar's recorded video are now uploaded in the [MAX dedicated Webpage](#) for the benefit of the users and on [MAX Youtube page](#) as well.

- ❑ The second [webinar](#) is dedicated to the AiiDA platform: "Managing, simplifying and disseminating High-Throughput computational materials science with AiiDA, AiiDA lab, and the Materials Cloud Archive" 27/05/2020 at 3 pm.

MAX WEBINARS

DATE: MAY 27 2020
TIME: 15.00 (CEST)

Managing, simplifying and disseminating High-Throughput computational materials science with **AiiDA**, **AiiDA lab**, and the **Materials Cloud Archive**.

SPEAKERS FROM EPFL

Sebastiaan Huber	Aliaksandr Yakutovich	Valeria Granata	Giovanni Pizzi
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AiiDA

max-centre.eu

The topics discussed during the webinar are:

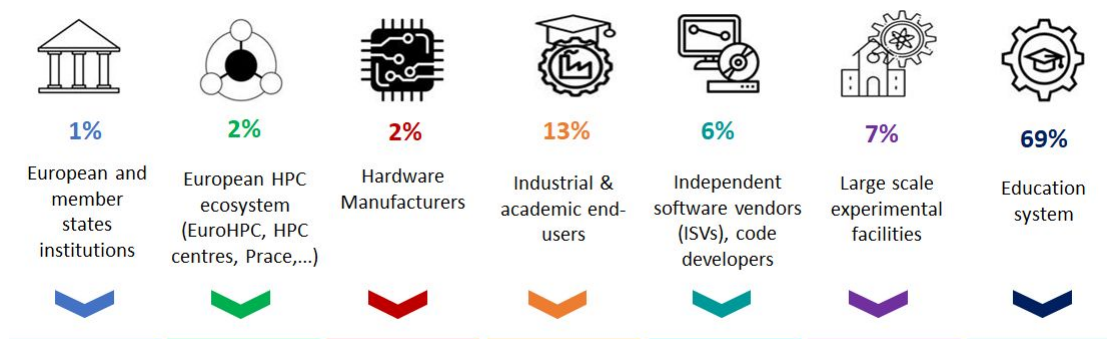
- How the MAX flagship code AiiDA supports its users to manage their computational workflows and the data that is produced,
- How AiiDA code can be used to automate workflows that directly employ the other MAX flagship codes, such as Quantum ESPRESSO,
- How AiiDA lab provides a user-friendly GUI to the workflows even for non-experts, and



- How the resulting data can easily be published through the Materials Cloud.

Speakers: Sebastian Huber (EPFL), Aliaksandr Yakutovich (EPFL), Valeria Granata (EPFL), Giovanni Pizzi (EPFL)

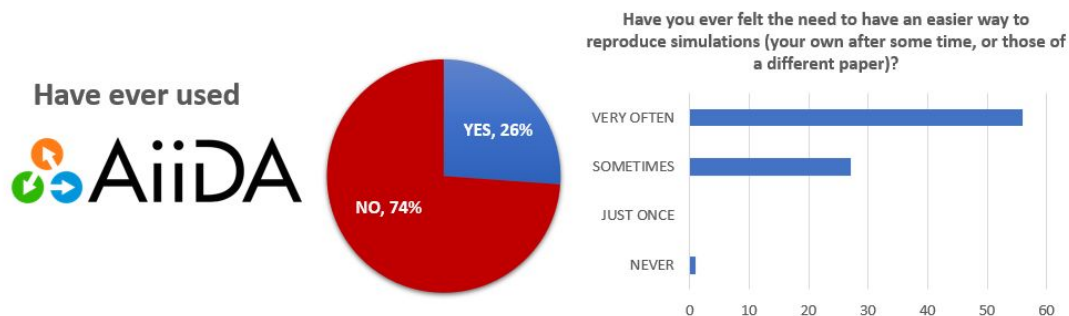
Attendance: **131 active participants** from



Registered people: 181 people.

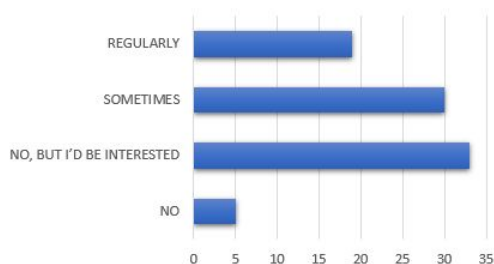
Interactions: **29 questions** were posed to the speakers.

Poll Questions: during the webinar we set **7 Poll Questions/Instant surveys** with these results

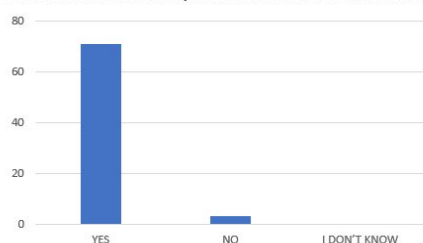




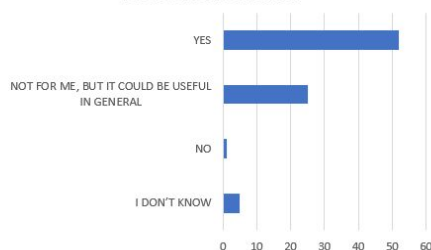
Do you run high-throughput simulations?



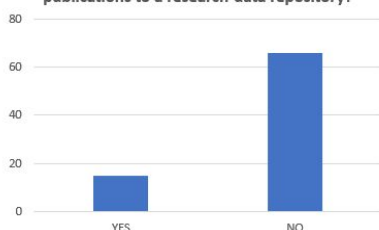
Do you think we need to have a platform that empowers collaborations between experimental or theoretical scientists?



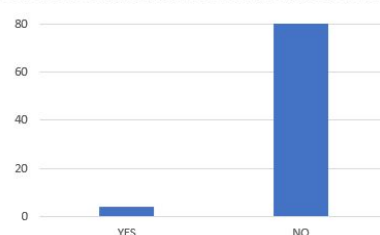
Do you think that a graphical user interface to AiiDA can be useful for researchers?



Have you ever submitted data associated to one of your publications to a research-data repository?



Have you ever submitted data to the Materials Cloud Archive?



❏ The series will continue with:

“Quasiparticle Band Structures and Excitons in Novel Materials using the Yambo Code” - 16/06/2020

“HPC libraries for CP2K and other electronic structure codes” - 24/06/2020

● MAX webinars in collaboration with Arm Research

April 16th and 18th, 2019

Arm Research, contributing to MAX "Co-Design" Work Package (WP4), organised two webinars on key technologies relevant to both WP4 objectives and EU Exascale plans. The first talk introduced the Arm Scalable Vector Extension (SVE) and the open-source gem5 simulation environment, tools that most researchers use for HW-SW design exploration. The



second talk provided an introduction to the Arm Instruction Emulator (ArmIE) and an associated methodology to evaluate the impact of SVE in the absence of SVE-enabled hardware. The co-design use-case presented was the High-Performance Conjugate Gradient (HPCG).

The aim is educating MAX partners interested in co-design of the next generation of High-Performance Computing systems, and hence disseminating and training MAX members to use freely accessible tools for HW-SW co-design.

Speakers: Filippo Spiga (ARM), Javier Setoain (ARM), Daniel Ruiz (ARM)

The recorded webinars are available in the [MAX training materials page](#).

- **Other online training activities:**

- The MAX EPFL node in collaboration with MARVEL organized the 3 public live webinars titled "[Fireside chats for lockdown times: A gentle introduction to density-functional theory](#)" by Nicola Marzari (EPFL) on [April 15-16-17, 2020](#). The webinar series was based on three conversations on the theory and the practice of DFT calculations, each 2 hours long, aimed either at experimental scientists that wanted to learn more about the field, or at researchers that wanted to start learning more about simulations. During the webinar the participants were able to type questions in the live chat; answers to the most topical ones were provided later in a PDF file. During the second day an introduction on how to set up density functional calculation in practice was organized by using the MAX flagship code Quantum ESPRESSO. In occasion of this handout the Quantum Mobile with pre-installed open-source MAX codes was made available. The event was a huge success reaching the limit of 500 subscriptions (the maximum number allowed by the platform) for all three days. The webinar videos were recorded and made [available](#) (together with the slides).
- Two MAX members - Daniele Varsano (CNR) and Zeila Zanolli (ICN) - participated to "[ETSF's Top Online Tutorials](#)". A selection of online tutorials (and related resources) in electronic structure and theoretical spectroscopy. MAX contribution to this joint initiative was to advertise the online course on [Computational Materials Physics](#) and [theoretical videolectures](#) and tutorials on the [Yambo code](#). Also, a virtual machine based on the Quantum Mobile was prepared and distributed. On [April 20th](#), an online question-and-answer webinar aimed to present the training material was organized with the presence of 18 subscribed participants.



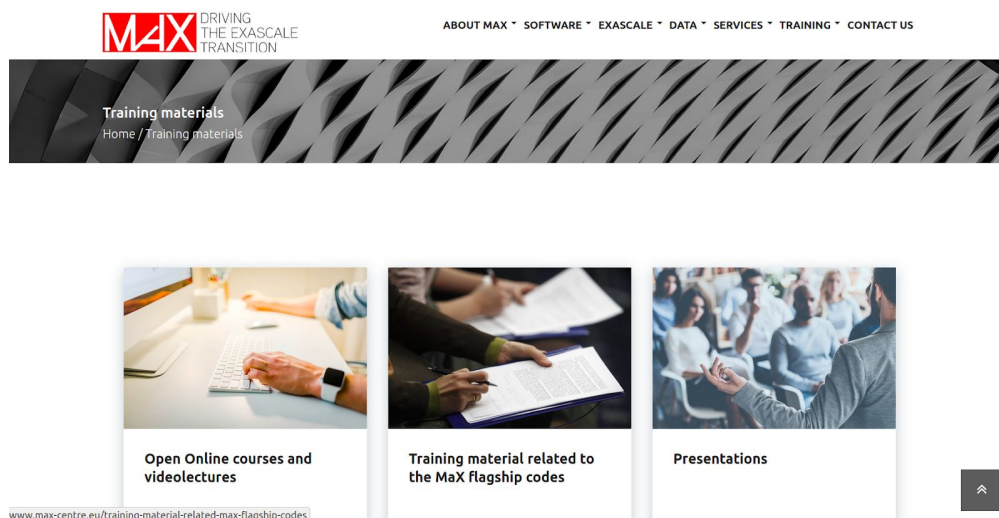
5 MAX strategy for online training

The MAX training plan and strategy was outlined in [D8.1](#) and it was based on a series of events where the training on flagship codes was delivered mainly in person with an important part of the training being dedicated to hands-on sessions. In the future we plan to continue along this line when there will be safe conditions to gather students and teachers. Nevertheless, based on the experience acquired in the last months in providing the training online (see webinar series, school on digital learning etc.), we plan to extend the future training offer of MAX *via* online training. Online events will permit to broaden the audience, remove travel barriers, and accept more students to single events overcoming logistic limitations as hall and lodging capacity. Based also in the feedback received in the occasion of the Virtual [School on Wannier90 v3.0](#) by AiiDA MAX team, here below we outline the preferable procedures for the next online training MAX events:

- A possible platform where to host the event is Zoom (up to 100 participants, even 500 with proper add-on).
- During the planning, it will be needed to find a compromise between prioritising the timezone of the speakers and maximising the presence of the attendees.
- All the lectures will be recorded and uploaded online - and made available for another portion of the audience.
- Q&A: the participants will be allowed to write their questions in a dedicated chat, while a moderator collects them in a document. The speakers can decide to answer on-the-fly or at the end of their talks. Offline, the speakers will answer questions, possibly gathering them by topic and integrating with the slide and the video of the talk: all the materials will be then available online.
- Hands-on tutorials: held virtually, as the participants can run tutorials on their own computers within the Quantum Mobile virtual machine.
- Tutors: the attendees can be personally helped online by the available tutors, without any interruptions for the speakers, and all the levels of experience on the topic can be easily covered



6 Repository of existing initiatives



All the training events organized by MAX were announced and advertised using community mailing lists, social media channels and the MAX [Newsletter](#). Announcements of the events, together with practical information were then collected in the [Training materials section](#) of the [new MAX website](#). Such a repository contains all the MAX and its partners' initiatives of interest to the computational materials research community. The online Training materials includes tutorials related to the MAX flagship codes, slides and presentations given during schools and tutorials and, most importantly, the video lectures recorded on occasion of recent and past schools, as well as the recent Webinars series on the MAX codes. This section offers the possibility to learn the theory at the base of the electronic structure calculations and the features implemented in the MAX flagship codes, and get practice with the use of the code by following remotely the online tutorials.

7 Conclusions

In the present Deliverable, we have described the MaX effort in providing specialised training and education in computational materials science both for end-users of MAX codes as well as to form a new generation of software developers in electronic structure and materials science. During the first period we have implemented the actions described in the Training and Education plan that was previously outlined in D8.1. Considering the COVID-19 pandemic MaX had to consider moving parts of its already organized events to online remote training and very likely this will be a solution also for future training activities.

All the training events organized for the MaX flagship code users and code developers (6 schools + 5 hackathons) were characterized by high participation of academic users and very



positive feedback on the organization and the provided training materials. These events were realized taking into account various priorities outlined in the training plan: the need of expanding the pan-European participation of users and institutions, as they were/will be organized in EU13 countries (paragraph 3.4); the use of the virtual machine Quantum Mobile, as it was highly encouraged many times (both in MaX schools and other events); the synergy in organizing events with other EU infrastructures, such as CECAM, Psi-k, PRACE and other CoEs and a particular attention to the gender balance both among participants and instructors.

While the academic users were highly attracted to the MaX training events, the industry engagement followed a different route: the “face-to-face” training that is strictly and specifically related to the needs of the customers (paragraph 3.4). MaX will pursue this method to enlarge the pool of such users.

MaX’s training offer is also built through the contribution of the MaX members in schools organized by other organizations on domain specific topics.

Importantly, MaX training offer was also devoted to undergraduate students contributing to teaching courses in Master programmes in Universities, for which good results and involvement are reported (paragraphs 3.6 and 3.7). More than 35 visiting students received training in MaX labs, pointing out the high interest of the community in MaX partners’ centres and in learning the usage of the flagship codes (paragraph 3.8).

The COVID-19 outbreak is changing deeply the way of delivering the training: during the lockdown, MaX contributed to various online training activities which provided the chance to experiment different formats (paragraph 4). In the present deliverable we have drafted a first strategy (paragraph 5) for future online training permitting to fulfill remotely important features of the MaX training programme as hands-on sessions, active participation and interaction with the users via user-focus group sessions. Hopefully the planned set up for online learning will allow to broaden the audience and accept more students to single events. The training material prepared on purpose for remote training, will be hosted in the training section of the MaX website (as already done for the in-person training) and will be a valuable resource of training also for interested users that could not attend the live events.



Appendix 1

Feedback from Tutorial on writing reproducible workflows for computational materials science *Venue and date: EPFL, Lausanne (CH). May 21-24, 2019*

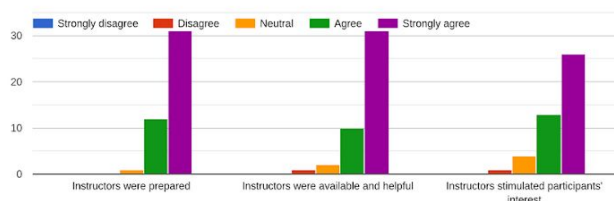
Organization of the tutorial



Tutorial impact on skills (only AiIDA part)



Skill and responsiveness of the instructors (only AiIDA part)



What aspects of this course were most useful or valuable?

- Hands on sessions with helpful experts available when needed
- The workflow.
- Understanding the new API. Using aiida vasp.
- - Hands-on tutorials with tutors being around for asking questions was very helpful to understand the general working principles of aiida and the querybuilder. - Jupyter notebook part was very good structured - Providing pre-configured machines: Best idea ever! (see below)
- Understanding the value of full provenance and structured data collection and preservation for calculations. Being in touch with developers to get introduced to AiIDA and the modules in a professional and guided way. Meeting other people working on similar topics to exchange ideas and expertise.
- Learning the basics of Aiida
- Workflow development
- How to use the QueryBuilder, different run options (run, submit), registering plugin
- plugin tutorials and setup instructions for development

How would you improve this course?

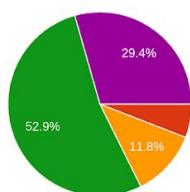
- By having more developer for the existing DFT code.



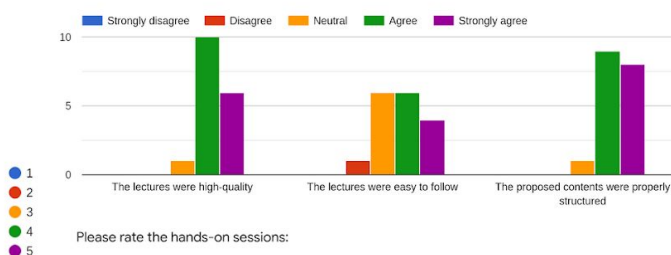
- I would focus less on the other topics that are not related to AiiDA directly. Particularly, I would prefer to hear more about AiiDA during the invited talks. Despite the other implementations of HPC are interesting to hear about, I expected to learn more about AiiDA itself during the lectures; not the other implementations.
- I would improve the tutorial with sessions where the participants try to solve "real/easy" problems (in group maybe).
- add an overview to the various aiiida objects
- Have an extended lecture at the end of the tutorial to put all the single parts together
- Focus more on the lectures and less on the hands-on/exercises
- More time to understand the concept and implementation of workflows. As an integral part of AiiDA it is very important. The time was not sufficient and the learning curve too steep to understand these concepts. Probably a more detailed explanation would also be good in the online guide.
- More time devoted to hands-on for workflows in specific plugins for those of us that are less keen on developing
- Very steep learning curve after the first 1.5 days for the first time AiiDA user

Feedback from One day Blender course Venue and date: CNR Nano, Modena (IT). June 27, 2019

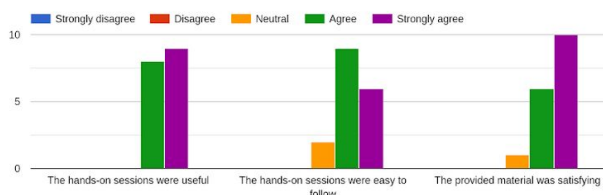
Overall evaluation (1-5) (1 Poor, 5 excellent)
17 responses



Please rate the lectures:



Please rate the hands-on sessions:



What aspects of this course were most useful or valuable?

- hand on and training material
- The hands on exercises, with clear objectives and a clear path to reach them. The files to start from were very useful.
- Making the user comfortable with the not-so-intuitive Blender UI
- To understand the possibilities of the software



- Animation hands-on session
- hot-keys, parenting objects, how to do simple animations

How would you improve this course?

- more time is needed to address the important topics of the course
- Focus a little bit more on actual use cases for scientific data.
- The course should be more focused on topics useful for scientific visualization. The lectures and topics covered could easily be found in online tutorials. The exercises were too many and too superficial. The lectures are very fast and difficult to follow. On the other hand some of the topics were in some cases not useful at all. I think to them it was not clear what we needed and/or we did not understand what they offered (a standard not tailored blender lecture)
- Due to the complexity of blender, I think that the course should be organised over two days
- Scripting session
- I would extend and give more details regarding data import from scientific packages, if possible also with more hands-on sessions.
- I would make it longer in time
- first part (morning) a bit slow, second part (afternoon) too fast. I would reduce the first part and focus better on the second part.
- Decrease the time dedicated to basic knowledge, improve time dedicated to more advanced features

Feedback from **Picking Fleur: hands on school Venue and date: Forschungszentrum Jülich, Jülich (DE). September 9-13, 2019**

If you have any general comments, criticism, or suggestions on how to improve any aspect of the workshop please provide them in the following lines:

- extremely good lectures
- Overall a very enjoyable and interesting school! Thank you all very much!
- competent, motivated team of lecturers / organizers
- thorough lectures on many-faceted topics
- easy-to-follow tutorials
- I am quite satisfied with the workshop. One thing that can be maybe added is a poster session
- with an individual discussion with the local experts about possibilities of collaborations.

The hands-on sessions were provided in two different approaches. We asked which approach they liked:

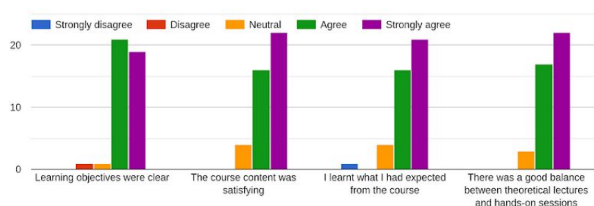
- Guided hands-on but with pauses for individual working is best – maybe mixed 50%/50%
- different approaches in tutorials; presented calculations (ok) vs. silent working + answering questions that arise (better)



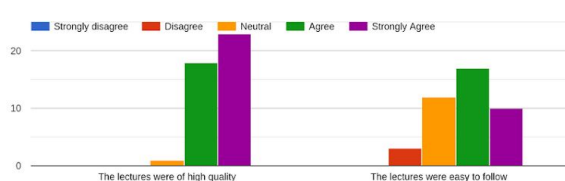
- In the tutorials sessions they are too fast which is very difficult to follow them. In contrast, the session on GW calculations was very good and also the first day

Feedback from **Computational School on Electronic Excitations in Novel Materials using the Yambo code** **Venue and date: ICTP Trieste (IT). January 27-31, 2020**

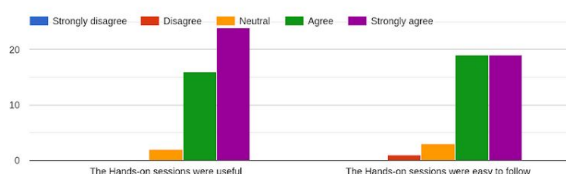
Course Content



Please rate the lectures



Please rate the Hands-on sessions

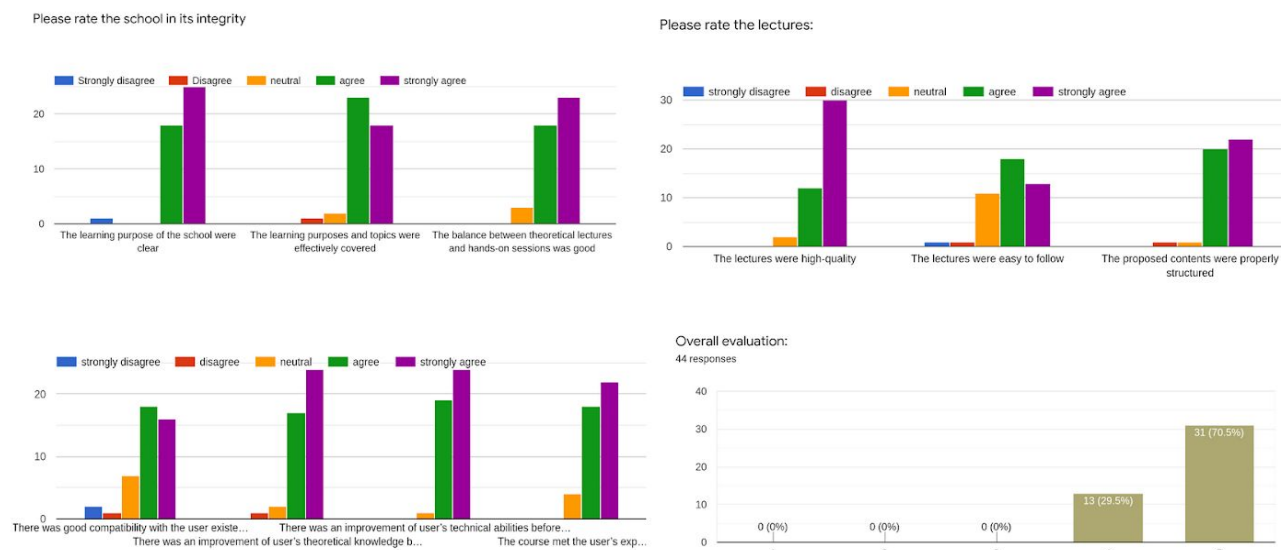


Any general comments, criticisms, or suggestions on how to improve any aspect of the school?

- The workshop was very well organized. I'd like to thank all organizers explicitly for creating a welcoming atmosphere and excellent learning environment
- The school should be organized more often
- All in all, a great school! The lecturers were extremely helpful and knowledgeable. I felt welcomed to ask questions at any time. Meeting new people from very diverse countries was an amazing experience. What I didn't like was a lack of bus connections to the city in the evening and the food on ICTP wasn't to my liking at all, sorry :-)
- The school was very helpful for me. Thanks to organizers for allow me to attend the school. I will like to attend more events like this in ICTP. ICTP stuffs are also very helpful. Overall a very nice experience.
- Perfect
- There was not enough time for all the tutorials and it was therefore sometimes hard to evaluate what we were actually doing, e.g. breaking down the calculations into single steps and corresponding command line options when generating the input file. The lectures helped a lot to understand the theory although some "low level" details were missing. On the other hand this can not really be avoided, taking into account time and the mixed background of the participants. Overall, this was a very good workshop, and it is very nice to have the presentations pdf's and recordings. Thank you!



Feedback from Summer School on Advanced Materials and Molecular Modelling with Quantum ESPRESSO *Venue and date: JSI, Ljubljana (SLO). September 16-20, 2019*



General comments, criticisms, or suggestions on how to improve any aspect of the event

- The school was very useful for people who were already basic users of QE, but a little hard to follow for people with no prior experience.
- One of the best Summer schools that I attended.
- I expected there would be at least a couple of hours dedicated to CPMD or MD capabilities of PW in general. Other than that everything was spot on. I applaud the inclusion of aida and GPU/HPC compilation/usage part of the course which was extremely useful and interesting.
- It was awesome, thank you very much. Maybe the only critic I could formulate would be about the work load, but it's not necessarily a problem. I must admit the last hands-on session on friday totally fried what was left of my brain and I couldn't work a lot more. In any case, congratulations for this summer school, I loved it and am pretty sure I learned a lot of useful things for my coming works and studies.
- The organization was beyond my expectation and I think it is worth emulating in subsequent schools of similar content.
- The lectures were too advanced and too fast. The exercises were very well prepared, but the physical background of the simulations (link to theory) was not clear. I would suggest reducing the scope of the material to explain the theory more slowly, repeat the theory during practice on one finished script and then give another physical problem to modify the script ourselves so we can't copy and paste what the instructions say without thinking.
- It was a balanced school but should have been at least 10 days programme and more topics related to TDDFT and few topics related to the recent studies should have been included. Overall it was good for beginners and very well organised school. Thank you!
- - Improvements: Hands on sessions should be at least 1-2 hour longer, with coffee break in between. Because at hands on, you can always expect some technical problems and it is



good to have more time. Maybe whole afternoon should be devoted to hands on, without any additional talks later in the evening. - Poster sessions were very good, although I am not fond of the the pitch part. I think the time for the pitch part could be better used with hands on sessions. Maybe the pitches would be only interesting for the winning poster. Also, I would suggest in the future not to only pick 1 winning poster, but maybe best 3, since I think there were a lot of nice works presented. - Theoretical lectures were excellent, all the lecturers did a great job! Congrats.



Appendix 2

List of researchers trained in CoE labs:

1) *Guest:* Dawson, William

Affiliation: RIKEN Japan

Hosting unit: CEA (FR) Luigi Genovese

Period: 18/03/2019 - 22/03/2019

Purpose of the visit: Fragment approach in BigDFT for the study of proteins

2) *Guest:* Fiscaro, Giuseppe

Affiliation: CNR Catane, Italy

Hosting unit: CEA (FR) Luigi Genovese

Period: 28/01/2019-01/02/2019

Purpose of the visit: Versatile boundary conditions for Poisson solver and convolutions

3) *Guest:* Saadat, Zahra

Affiliation: Sharif University of Technology, Teheran

Hosting unit: CNR (IT) - Elisa Molinari

Period: 19/09/2019-16/12/2019

Purpose of the visit: HPC-Europe3 visit. Training on HPC environment and scientific support for the first principles investigation of transition-metal dichalcogenides heterostructures.

4) *Guest:* Caldas, Marilia J.

Affiliation: Dep.to de Fisica dos Materiais - Instituto de Fisica Universidade de São Paulo (USP) Brasil

Hosting unit: CNR Nano, Modena (IT) - Elisa Molinari

Period: 01/01/2019 - 28/02/2019

Purpose of the visit: properties of hybrid organic/inorganic interfaces, and electronic properties of 2-D materials electronic and optical properties of defects in oxides

5) *Guest:* Valencia, Ana Maria

Affiliation: Dep.to de Fisica dos Materiais Instituto de Fisica - Universidade de São Paulo (USP) - Brasil

Hosting unit: CNR Nano, Modena (IT) - Elisa Molinari



Period: 14/01/2019 - 20/01/2019

Purpose of the visit: Studies of 2-D materials

6) *Guest:* Caldas, Marilia J.

Affiliation: Dep.to de Fisica dos Materiais - Instituto de Fisica Universidade de São Paulo (USP) Brasil

Hosting unit: CNR Nano, Modena (IT) - Elisa Molinari

Period: June 2019

Purpose of the visit: properties of hybrid organic/inorganic interfaces, and electronic properties of 2-D materials electronic and optical properties of defects in oxides

7) *Guest:* Vitale, Valerio

Affiliation: Imperial College London, UK

Hosting unit: EPFL (CH) - Giovanni Pizzi

Period: 28/01/2019 - 28/01/2019

Purpose of the visit: Robust automatic wannierization

8) *Guest:* Gebreyesus, Gebremedhn

Affiliation: College of Basic and Applied Sciences, University of Ghana, and College of Natural Science, Addis Ababa University, Ethiopia

Hosting unit: EPFL (CH) - Nicola Marzari

Period: 03/02/2019 - 09/02/2019

Purpose of the visit: Hubbard-corrected density-functional theory for studies of structural and electronic properties of perovskites.

9) *Guest:* Ruchika, Mahajan

Affiliation: Indian Institute of Technology Mandi, India

Hosting unit: EPFL (CH) - Giovanni Pizzi

Period: 20/05/2019 - 25/05/2019

Purpose of the visit: AiiDA, DFT+U

10) *Guest:* Marcel Sadowski

Affiliation: Technical University Darmstadt, Germany

Hosting unit: EPFL (CH) - Nicola Marzari

Period: 01/04/2019 - 30/06/2019



Purpose of the visit: Investigations on mixed layered transition metal oxides $\text{Li}(\text{Ni}, \text{Co}, \text{Mn})\text{O}_2$ with DFT+U calculations.

11) *Guest:* Dewandre, Antoine

Affiliation: University of Liege, Belgium

Hosting unit: ICN2 (ES) - Pablo Ordejon

Period: 26/12/2018 - 21/12/2018

Purpose of the visit: Thermal properties of Dichalcogenide stacked heterostructures and Ferrecrystals

12) *Guest:* Melo, Pedro

Affiliation: University of Liege, Belgium

Hosting unit: ICN2 (ES) - Pablo Ordejon

Period: 26/12/2018 - 21/12/2018

Purpose of the visit: Exciton and defect dynamics on WSe_2 and MoS_2 , and their impact in real-time dynamics

13) *Guest:* Dilson, Juan

Affiliation: CONICET-CNEA, Argentina

Hosting unit: ICN2 (ES) - Pablo Ordejon

Period: 21/01/2019 - 07/02/2019

Purpose of the visit: Oxygen migration barriers in complex oxides, and spin-orbit effects in manganites.

14) *Guest:* Dewandre, Antoine

Affiliation: University of Liege, Belgium

Hosting unit: ICN2 (ES) - Pablo Ordejon

Period: 01/04/2019 - 27/04/2019

Purpose of the visit: Thermal properties of Dichalcogenide stacked heterostructures and Ferrecrystals

15) *Guest:* Melo, Pedro

Affiliation: University of Liege, Belgium

Hosting unit: ICN2 (ES) - Pablo Ordejon

Period: 01/04/2019 - 27/04/2019



Purpose of the visit: Exciton and defect dynamics on WSe₂ and MoS₂, and their impact in real-time dynamics

16) *Guest:* Pouget, Jean Paul

Affiliation: Université de Paris-Sud, Université Paris-Saclay, France

Hosting unit: ICN2 (ES) - Pablo Ordejon

Period: 21/04/2019 - 23/04/2019

Purpose of the visit: Electron/spin-lattice coupling in low dimensional organic conductors

17) *Guest:* Bristowe, Nicholas

Affiliation: University of Kent, UK

Hosting unit: ICN2 (ES) - Pablo Ordejon

Period: 23/06/2019 - 12/07/2019

Purpose of the visit: Multiferroic materials, and spin-orbit effects at interfaces of complex oxides.

18) *Guest:* Castillo, José María

Affiliation: Universidad Nacional Autónoma de México, Mexico

Hosting unit: ICN2 (ES) - Pablo Ordejon

Period: 02/05/2019 - 31/07/2019

Purpose of the visit: magnetic nanoparticles and thermal properties

19) *Guest:* Oroszlanyq, Laszlo

Affiliation: Eötvös Loránd University, Hungary

Hosting unit: ICN2 (ES) - Pablo Ordejon

Period: 12/12/2019 - 13/12/2019

Purpose of the visit: Implementation Force-theorem to compute J's with SIESTA-SOC

20) *Guest:* LoPiccolo, Mattia

Affiliation: University of Palermo

Hosting unit: ICN2 (ES) - Pablo Ordejon

Period: 07/01/2020 - 29/02/2020

Purpose of the visit: ab initio MD simulations of amorphous silica



21) *Guest:* Dieguez, Oswaldo

Affiliation: Tel Aviv University

Hosting unit: ICN2 (ES) - Pablo Ordejon

Period: 01/09/2019 - 31/08/2020

Purpose of the visit: Order-N methods

22) *Guest:* Hassan, Ahmoum

Affiliation: LP2MS, Moulay Ismail University, Faculty of Sciences, Meknes Morocco

Hosting unit: ICTP, Trieste, Italy (IT) - Ralph Gebauer

Period: 04/02/2019 - 27/04/2019

Purpose of the visit: Discovering the magnetic and thermoelectric properties of (Ni,Co) codoped ZnO nanowire with and without the presence of defect

23) *Guest:* Shick, Alexander

Affiliation: Institute of Physics, ASCR, Prague, Czech Republic

Hosting unit: JUEL (DE) - Stefan Blügel

Period: 14/03/2019 - 22/03/2019

Purpose of the visit: Implementation of the Hubbard 1 model

24) *Guest:* Nandy, Ashis Kumar

Affiliation: School of Physical Sciences, NISER Bhubaneswar, India

Hosting unit: JUEL (DE) - Stefan Blügel

Period: 21/05/2019 - 21/07/2019

Purpose of the visit: Training on the treatment of semiconductor interfaces with Fleur

25) *Guest:* Tas, Murat

Affiliation: Altinbas University, Istanbul, Turkey

Hosting unit: JUEL (DE) - Stefan Blügel

Period: 08/07/2019 - 03/08/2019

Purpose of the visit: GW investigations on WTe₂

26) *Guest:* Katsumoto, Hiroshi

Affiliation: Osaka University, Osaka, Japan

Hosting unit: JUEL (DE) - Stefan Blügel

Period: 05/10/2019 - 19/10/2019



Purpose of the visit: Usage of FLAPW in the context of multiferroics

27) *Guest:* Nanavati Sachin

Affiliation: Cardiff University, Cardiff, UK

Hosting unit: JUEL (DE) - Stefan Blügel

Period: 17/10/2019 - 20/11/2019

Purpose of the visit: Optimization of computationally expensive kernels on GPUs

28) *Guest:* Juan Manuel Radear

Affiliation: Tecnologico de Monterrey, Campus Ciudad de Mexico, Mexico

Hosting unit: UGENT (BE) - Stefaan Cottenier

Period: 07/05/2019 - 23/5/2019

Purpose of the visit: use of QE for magnetocrystalline anisotropy energy

29) *Guest:* Rita Omamuyovwi Akemu

Affiliation: University of Benin, Nigeria

Hosting unit: UGENT (BE) - Stefaan Cottenier

Period: 05/12/2019 - 13/2/2020

Purpose of the visit: phonon calculations with QE

30) *Guest:* Fujiwara Ikki

Affiliation: National Institute of Informatics, Japan

Hosting unit: EPFL (CH) - Giovanni Pizzi

Period: 18/06/2019

Purpose of the visit: Discussion on AiiDA, motivations, and policies

31) *Guest:* Takaaki Aoki

Affiliation: Kagawa University, Japan

Hosting unit: EPFL (CH) - Giovanni Pizzi

Period: 18/06/2019

Purpose of the visit: Discussion on AiiDA, motivations, and policies

32) *Guest:* Muechler Lukas



Affiliation: Flatiron Institute

Hosting unit: EPFL (CH) - Nicola Marzari

Period: 26/08/2019 - 28/08/2019

Purpose of the visit: Machine Learning

33) *Guest:* Bölle Felix

Affiliation: Technical University of Denmark

Hosting unit: EPFL (CH) - Giovanni Pizzi

Period: 07/10/2019 - 13/12/2019

Purpose of the visit: Understanding and trying to enhance the existing ASE/GPAW plugin

34) *Guest:* Warren James

Affiliation:

Hosting unit: EPFL (CH) - Giovanni Pizzi

Period: 27/01/2020 - 28/01/2020

Purpose of the visit: Discussion on AiiDA.

35) *Guest:* Hiriyama Motoaki

Affiliation: RIKEN Center for Emergent Matter Science

Hosting unit: EPFL (CH) - Giovanni Pizzi

Period: 10/02/2020 - 14/02/2020

Purpose of the visit: Discussion on AiiDA.

36) *Guest:* Klaus Dieterich

Affiliation: Bosch Research Foundation

Hosting unit: 26/02/2020 - 27/02/2020

Period: EPFL (CH) - Nicola Marzari

Purpose of the visit: Industrial collaboration with Bosch

37) *Guest:* Stephen Wu

Affiliation: Institute of Statistical Mathematics, Japan

Hosting unit: EPFL (CH) - Leopold Talirz

Period: 08/04/2020 (zoom, due to Corona)



Purpose of the visit: Integration of XenonPy ML platform with AiiDA

38) *Guest:* Chang Liu

Affiliation: Institute of Statistical Mathematics, Japan

Hosting unit: EPFL (CH) - Leopold Talirz

Period: 08/04/2020 (zoom, due to Corona)

Purpose of the visit: Integration of XenonPy ML platform with AiiDA

39) *Guest:* Souza Ivo

Affiliation: Centro de Física de Materiales, Universidad del País Vasco

Hosting unit: EPFL (CH) - Nicola Marzari

Period: 16/10/2019 - 18/10/2019

Purpose of the visit: Quantum ESPRESSO and the AiiDA-Wannier90 workflows