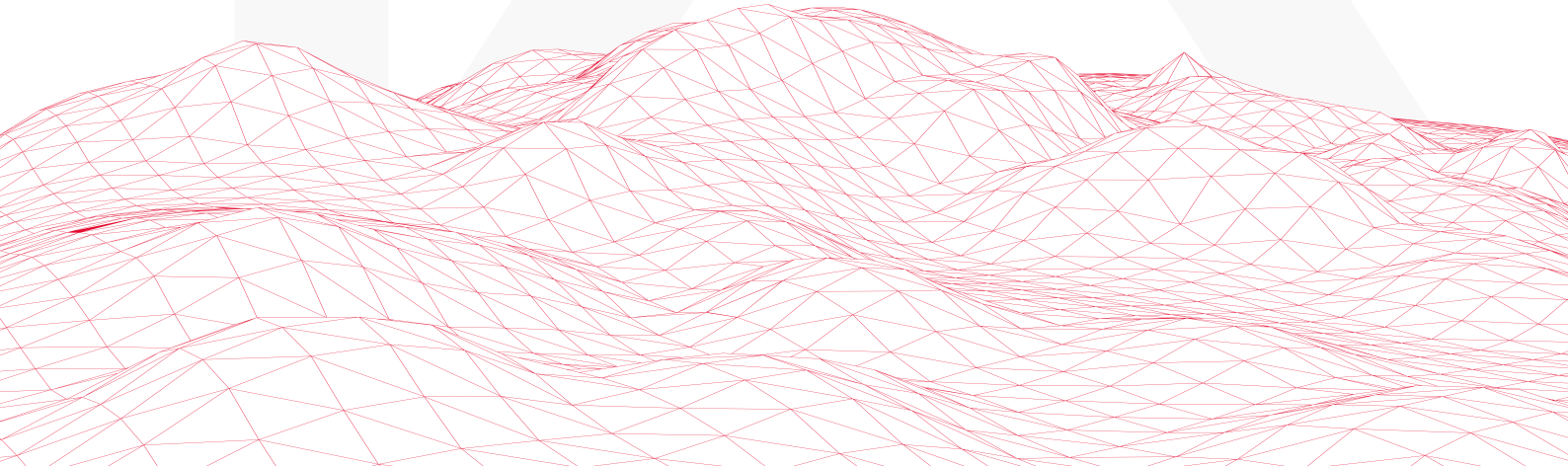
MAX DRIVING THE EXASCALE TRANSITION

max-centre.eu

MAX online training on codes: material & links



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The training activities was a collective enterprise of MAX partners.
Editorial editing and content supervision: Maria Celeste Maschio, Maria Bartolacelli, Luisa Neri, and MAX Management Team.
Technical and graphical realization: Trust-IT Services.

Introduction

*The **MAX Centre of Excellence**, since its inception, has placed the training of the new generation of code developers and of code users at the core of its activities. Thus, a great effort has been put in this direction as shown by the large number of schools organized in the last years.*

Starting from February 2020, due to the limitations related to the COVID19 pandemic, the modalities of the training offer have profoundly changed: consequently the entire training activity of MAX has been reshaped in order to organize schools and hackathons only on online digital platforms.

These changes have required a great deal of effort both from teachers, who had to learn new ways of delivering training, and above all from students, who had to give up all the benefits of in-person learning, such as direct contact with tutors and the opportunity to collaborate with their colleagues.

On the other hand, online training activities helped remove travel barriers, overcome logistical limitations, and expand the audience of students. Nonetheless, they required the preparation of plenty of online training material, that remains available beyond the time of schools, and is conveniently within everyone's reach.

In this booklet, the reader will find the collection of all the online events organized by MAX in 2021, mainly focused on the theory, implementations, and use of the most used MAX flagship codes (Quantum ESPRESSO, Siesta, Yambo, Fleur, AiiDA) in the HPC environment.

For each school, a dedicated section describes the organization and the main objectives of the event: users will find all the links to the available material prepared by the MAX trainers, such as the complete recording of the lectures, the slides, and the online tutorials that students can follow at their own pace.

The training activity is developed along MAX Action 4 "Widening the access to codes and fostering transfer of know-how to user communities" and deployed by Work Package 8. The excellent feedback received from students make us believe that it is of very strong interest and value beyond the project for the growth of expertises in a very seminal field.

Daniele Varsano (CNR Nano)
Coordinator of MAX Training and Education

MAX school on advanced materials and molecular modelling with Quantum ESPRESSO

17th - 28th May 2021

The school introduced students and young researchers to materials and molecular modelling with Quantum ESPRESSO (QE), covering basic concepts, recent advances and developments, with emphasis on density functional theory (DFT) based methods and High Performance Computing (HPC).

Computational methods in electronic structure theory are a powerful tool for the understanding and the prediction of materials properties at the atomistic level. The combination of the progress made by condensed matter theory with the increasing computing capabilities provided in HPC centers fosters a great interest in computational materials science. Ab-initio electronic structure software like QE makes such potentialities easily available to a wide audience of scientists and students.

The purpose of this school was to introduce students and young researchers to materials and molecular modelling with QE. The school aimed to train beginners in computational materials sciences to the efficient use of QE on modern massively parallel architectures, with special emphasis on the emerging architectures based on GPGPUs and on the use of advanced tools for generating, managing, storing, and sharing results.

Organizers: Stefano Baroni (SISSA), Ralph Gebauer (ICTP), Anton Kokalj (Jožef Stefan Institute), Wei Ren (Shanghai University), Alessandro Stroppa (CNR-SPIN), with a strong support by the local organizers Ivan Girotto (ICTP) and Ivan Carnimeo (SISSA).

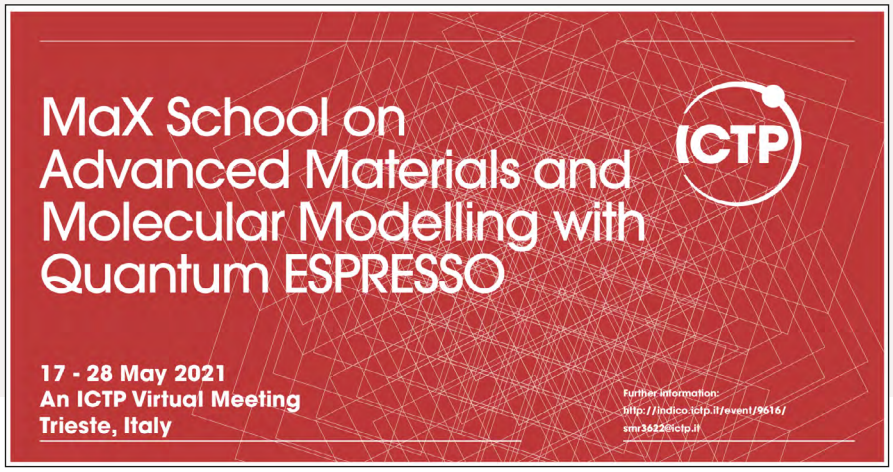
There was no registration fee.

More details in the MAX news

In collaboration with:

Additional links

Quantum ESPRESSO and MAX
Quantum ESPRESSO Official Page



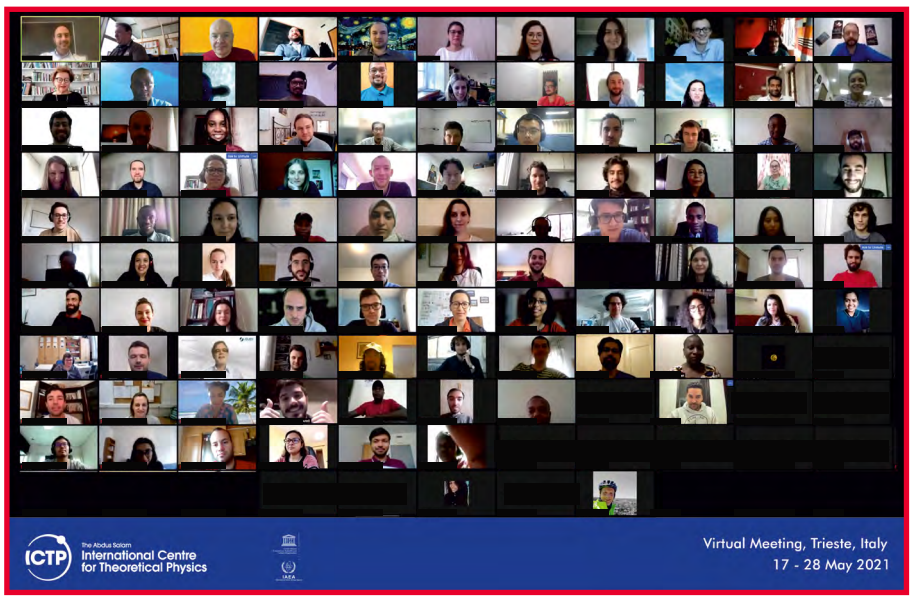
Report

The school was virtually hosted at the ICTP centre, Trieste (IT), on 17th-28th May 2021 with an innovative two-week school program: the lectures were held in the mornings (CEST) followed by hands-on sessions. In this way, the chosen time-window allowed students and researchers from Far-East and South-East Asia to attend the school in real-time. In order to permit the students from a different time zone (USA, for example) to attend the lectures, the entire school was video-recorded and it is now available on the web.

The school was highly appreciated world-wide, with a record-breaking number of applicants (1292), as far as ICTP virtual activities are concerned (since Feb 2020). For technical reasons, only about 120 participants were finally selected to attend the online school, with special attention paid to gender and nationality balance. However, applicants who were not selected as participants, could attend the school in streaming on the MaX Youtube channel.

Features of the school particularly appreciated by the virtual audience were: the adoption of a Virtual Machine (VM) for the e-laboratories, i.e., a uniform environment based on Ubuntu Linux that comes with a collection of quantum simulation codes (Quantum ESPRESSO, Xcrysden package, and others) and the 24/7 possible interaction with faculties and tutors. Every participant could install the VM on their own laptop for the hands-on sessions, and was able to interact with the school staff either on Zoom during online sessions but also via dedicated slack channels created on purpose, where school staff and participants could interact despite the different time zones. Furthermore, advanced exercises were run on five different HPC clusters seen by the users as a sort of unified cloud platform, i.e., Ulysses (SISSA), Argo (ICTP), Arnes (ARNES), Marconi-100 (CINECA), and HZW tech Cloud computing.

LECTURES **SPECIAL GUESTS LECTURES**



SISSA

ICTP The Abdus Salam International Centre for Theoretical Physics

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Advanced school on Quantum Transport using SIESTA

17th - 21st May 2021

This five-day online school focused on the field of theoretical condensed matter electronic transport exploiting the non-equilibrium Green's function approach. In particular, recent advances in transport theory were presented in the form of lectures and hands-on sessions on hot topics in the field. The teachers presented novel methods used for materials research modelling.

The participants learnt the advanced features of SIESTA, such as the calculations of non-equilibrium properties using the TranSIESTA/TBtrans approach and the python framework SISL. For example, the school lectures covered a recent scheme introducing truly single-junction transport calculations and the new implementations to include in the transport calculations different corrections to the Hamiltonian accounting for electron-phonon coupling, spin orbit coupling, and electronic correlation. Moreover, the users learnt how to extract a tight-binding Hamiltonian from a DFT Hamiltonian allowing them to deal with very large systems.

Organizers: Simona Achilli (University of Milan), Mads Brandbyge (Technical University of Denmark, Lyngby), Thomas Frederiksen (DIPC - Donostia International Physics Center), Pablo Ordejon (ICN2, Catalan Institute of Nanoscience and Nanotechnology), Nick Papior (Technical University of Denmark), Zeila Zanolli (Utrecht University).

There was no registration fee.

More details in the MAX news

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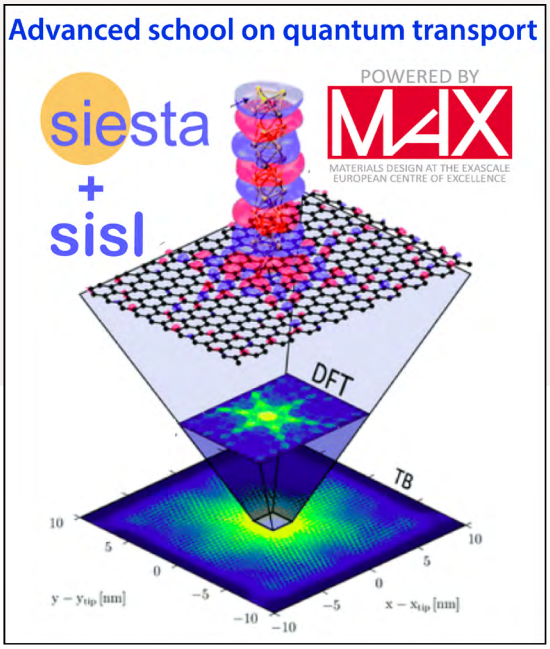
DIPC Donostia International Physics Center

Additional links

SIESTA and MAX
SIESTA Official Page



Report

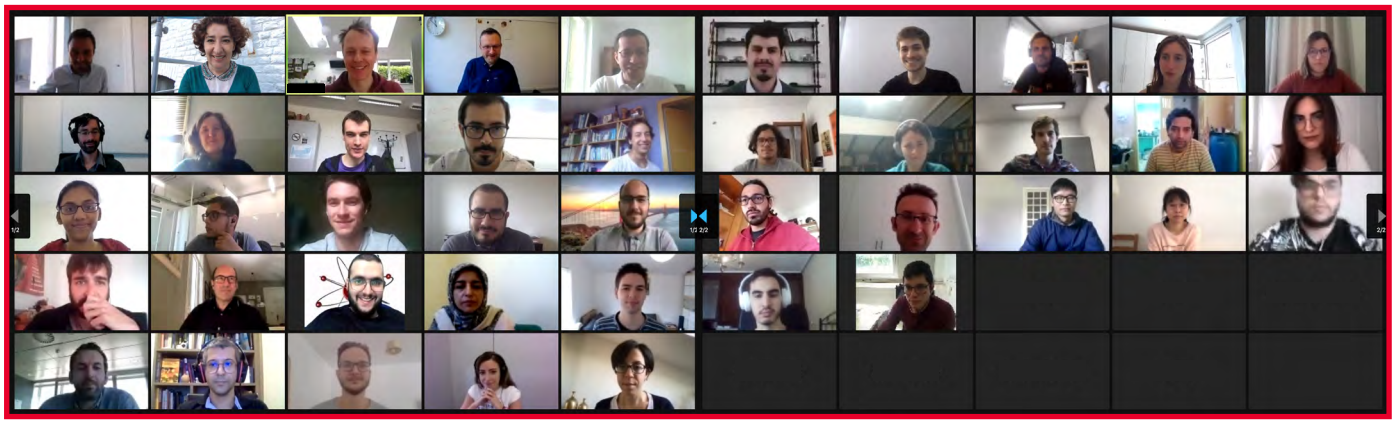
This five-day online school, held on 17th-21st May 2021, supported by CECAM, was focused on the field of theoretical condensed matter electronic transport exploiting the non-equilibrium Green's function approach. Theoretical lectures covering hot topics of the field and advanced features of the code were held live in the morning via Zoom. The registrations were uploaded daily in the Youtube channel of the school.

Hands-on sessions in the afternoon were performed by the users on their local machine with the live support of tutors via the platform Discord. This allowed an efficient organization of the tutorials, performed step by step with increasing order of difficulty. In addition, the users also had the opportunity to interact with each other and to get involved in the community of the code developers which is currently active in the Discord channel shared during the school. The SIESTA code was supplied via a Virtual Machine, and the Jupyter Notebook was used for the SISL Python scripts.

The workshop also hosted an afternoon online poster session, organized through Zoom rooms, to which all participants were invited to present and discuss their various research projects.

The satisfactory survey gave 60% of the users extremely satisfied about the school format, topics treated and sharing of materials.

LECTURES **TUTORIALS**



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First-principles simulations of materials with SIESTA

28th June - 2nd July 2021

The school was aimed at students and researchers from different disciplines who would already use, or would plan to use, first-principles techniques to simulate properties of matter at the atomic scale. In particular, the school focused on the SIESTA method. Participants learnt its essential theoretical foundations, and how to use the SIESTA code effectively.

Pre- and post-processing tools were also presented. The format of the school (completely online) allowed for a flexible offering of modules of different levels, from basic to advanced, so that participants could adapt their syllabus. In addition, the material prepared for the school was integrated into the corpus of SIESTA documentation, which remains available for continuous learning.

An online support forum was open before, during, and for some time after the canonical school dates to provide further guidance, to answer questions, and to facilitate discussions between school students and tutors.

Organizers: Emanuele Bosoni (ICMAB-CSIC, Institut de Ciencia de Materials de Barcelona), Antonio Cammarata (Czech Technical University in Prague), José María Escartín Esteban (ICN2, Catalan Institute of Nanoscience and Nanotechnology), Alberto Garcia (ICMAB-CSIC, Institut de Ciencia de Materials de Barcelona), Pablo Ordejon (ICN2), Miguel Pruneda (ICN2), Zeila Zanolli (Utrecht University).

There was no registration fee.

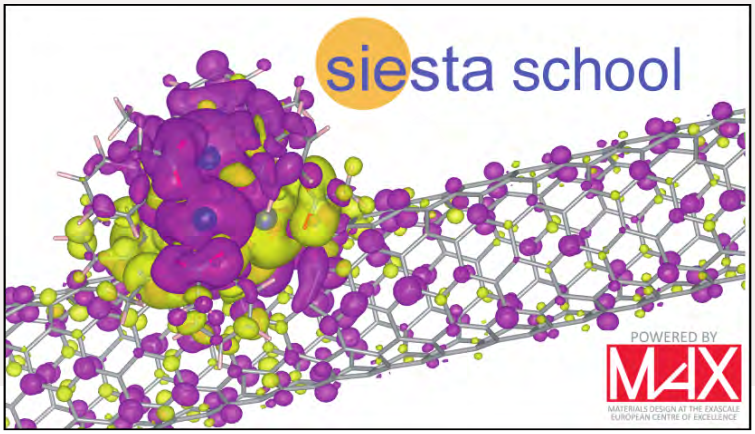
More details in the MAX news

In collaboration with:

cecam
Centre Européen de Calcul Atomique et Moléculaire

Additional links

SIESTA and MAX
SIESTA Official Page



Report

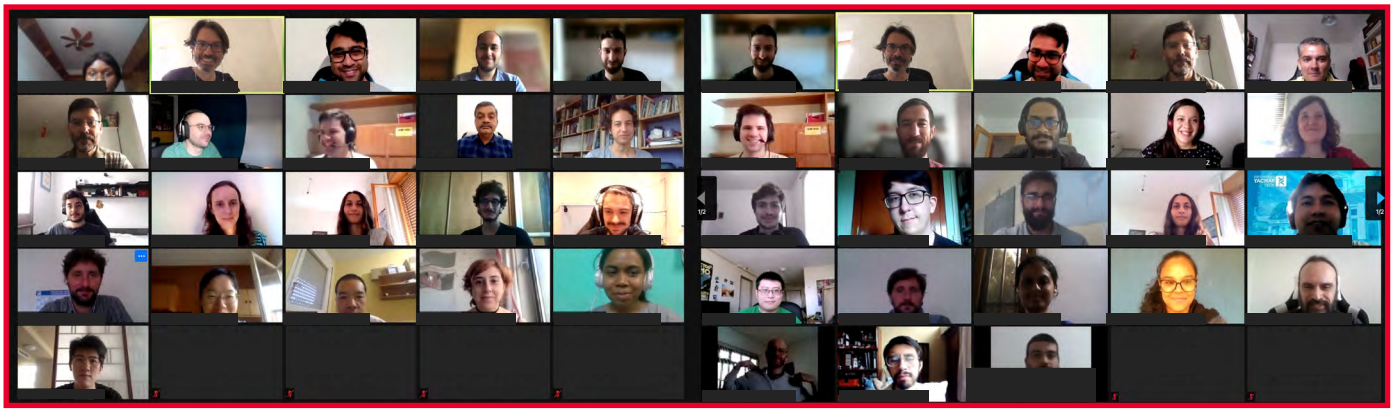
The purpose of this online CECAM school was to present the fundamentals of SIESTA to novel users, as well as to provide advanced training on topics other than quantum transport (already covered by the Advanced School) to users with intermediate and advanced skills. Out of 263 applicants, 104 diverse participants were selected upon their potential.

Over a third of participants had never used SIESTA before, another third had some basic skills, and the remainder had intermediate to advanced skills. The week before the school saw the release of a set of pre-recorded lectures on the SIESTA YouTube channel – this gave the students the time to watch the videos at their own pace– and of a new virtual machine –so that students could run SIESTA and the other required tools from almost any computer. Finally, during the week of the school (28th June - 2nd July 2021), we ran two tracks of live hands-on tutorials (9:30-12:30 and 16:00-19:00 CEST everyday) in order to adapt to the range of time zones of the participants.

The school tutorials (many designed for the occasion) were available on a new readthedocs site. All participants could choose, based on their skills and interests, whether to follow a proposed stream of basic tutorials, or to work on the scheduled advanced tutorial –specialised tutors had been arranged for every 90 minute block. Almost all discussions took place on a discord server, where chat rooms had been allocated to discuss each of the individual tutorials.

Even though most participants had never used discord or a virtual machine, they seemed to adapt well to them, and throughout the week there was a sustained level of engagement and learning. The feedback received was very positive, in particular about the quality of the tutorial materials and of the tutors. A large majority of the respondents reported that the school qualitatively improved their SIESTA skills, and would definitely recommend the school to colleagues.

LECTURES **SLIDES** **TRAINING MATERIAL**



ICN2 Institut Català de Nanociència i Nanotecnologia

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Virtual school on "Electronic excitations in solids and nano-structures using the Yambo code"

8th - 9th / 15th - 16th April 2021

The MaX/CECAM virtual school was held on 8th-9th April (week 1) and 15th-16th April (week 2) 2021 using the online platform Zoom.
The school aimed to introduce participants to post-DFT simulations, in particular to many-body perturbation theory (MBPT) approaches and provided both theoretical overviews and practical training on the calculation of electronic and optical properties of solids and nanostructures.

Participants attended theoretical lessons on Many-Body Perturbation Theory - organised in short modules - that introduced them to the concepts based on the linear response, GW and Bethe-Salpeter calculations. A strong focus was put on the connection with experimental observables (from photoemission to absorption and photoluminescence). Dedicated online hands-on sessions were held for each topic, to gain experience and directly learn the use of the Yambo code. Students further learnt how to run post-processing tools for the analysis of the results.
Participants were required to have a background in DFT methods, including experience in running first-principles simulations.

Organizers: Myrta Grüning (Queen's University Belfast), Conor Hogan (ISM-CNR, Institute of Structure of Matter), Maurizia Palummo (University of Rome Tor Vergata), Daniele Varsano (CNR Nano)

There was no registration fee.

More details in the MAX news

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cecam Centre Européen de Calcul Atomique et Moléculaire

Consiglio Nazionale delle Ricerche

Additional links

Yambo and MAX
Yambo Official Page

Report

The school was sponsored by CECAM and was held in virtual form, due to the pandemic situation, taking advantage of Zoom, YouTube (two channels), Slack, the Yambo website, and providing pre-installed software via Docker images and/or a dedicated virtual machine. The school lasted four days split over two weeks with the participation of more than 130 students from 35 different countries.

Theoretical lectures were held in the morning (CEST) and the video recordings of the lectures were immediately uploaded to the Yambo website and MaX youtube channels. Question/Answer sessions were allocated after each talk. The afternoons were dedicated to hands-on tutorials. Before the school all the participants received information about the installation of the Yambo code with multiple choices, including instructions on how to install the code on their machines, the possibility to download a Virtual Machine containing the code and the files needed for the tutorials, or instructions to set up a Yambo container through the docker platform.

Tutorials were made available via wiki pages and the attendees were grouped in different break-out rooms where a tutor (one every five/six people) was present to guide the attendees through the exercises and to answer their questions. Replies to satisfaction questionnaires showed that about 69% of participants were extremely satisfied and 27% satisfied with the event.

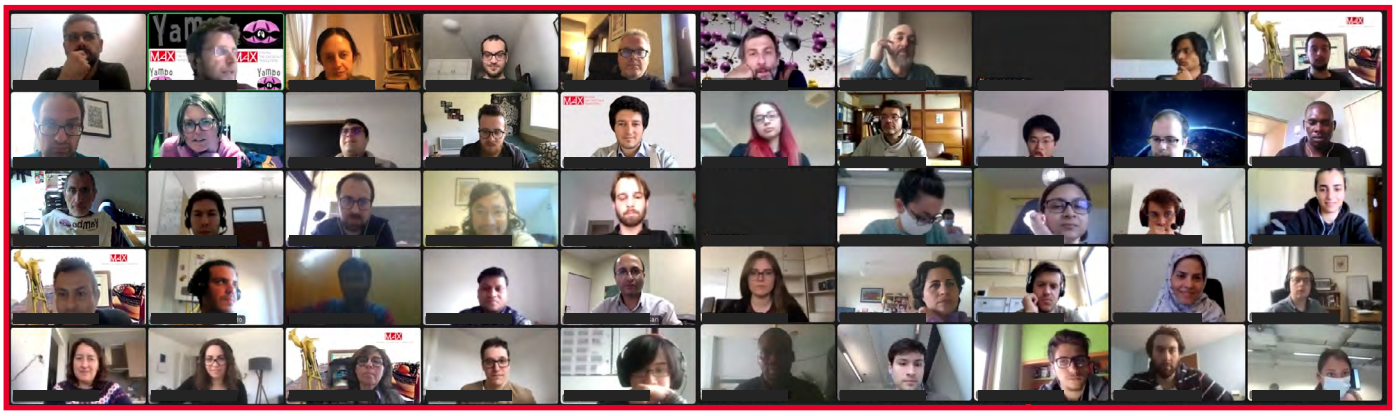
LECTURES **TUTORIALS**

More on past training events

2020 School

MAX news

LECTURES **TUTORIALS**



Consiglio Nazionale delle Ricerche

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www.flapw.de

fleur

Picking Flowers - Online Hands-on Tutorial

12th - 16th April 2021

The density-functional theory (DFT) in its various incarnations provides the most practical framework to compute basic electronic, magnetic, and structural properties of materials. Large scale materials screening using DFT is believed to be a key factor in future materials development. The full-potential linearized augmented planewave (FLAPW) method has emerged as a robust and precise state-of-the-art technique with reasonable computational efficiency. It is widely accepted as providing the reference solution.

However, the use and application of DFT methods and of FLAPW in particular require a thorough training where users meet developers of such methods. Hence this tutorial focuses on training the participants in using our all-electron FLAPW DFT code FLEUR. A special focus will be on 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.

Our school consisted of lectures covering three main areas:
- the underlying basic theory;
- the installation and usage of FLEUR and its AiiDA interface;
- more specialized topics relevant for typical FLEUR calculations.

Organizer: Daniel Wortmann (Forschungszentrum Jülich)

There was no registration fee.

More details in the MAX news

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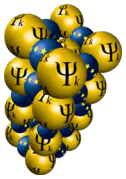
Centre Européen de Calcul Atomique et Moléculaire



Additional links

FLEUR and MAX
FLEUR Official Page

www.flapw.de

Picking Flowers:
Online Hands-on
Tutorial
12.4.21-16.4.21

Report

The FLEUR workshop covered the basic usage of the code and also its combination with the SPEX code for GW calculations and with an AiiDA infrastructure to enable high-throughput projects. A special focus was placed on the calculation of magnetic properties.

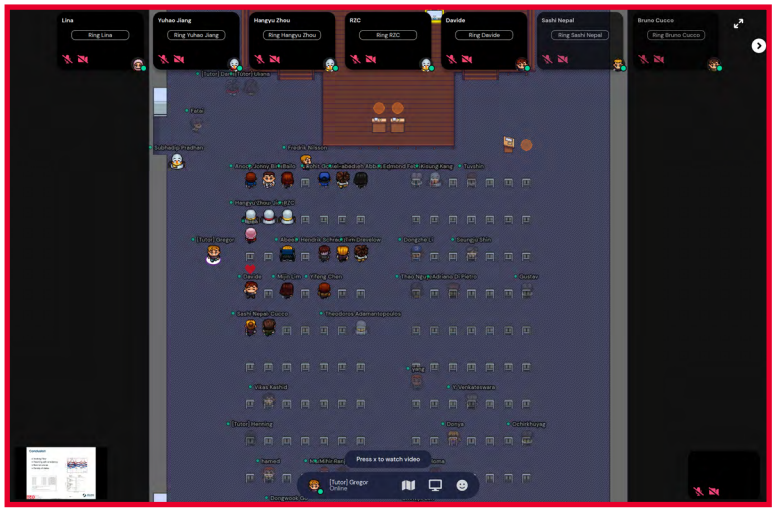
The workshop was held in a purely virtual setup on 12th-16th April 2021, offering different participation options. The default participation was based on an integrated Gather.Town environment. It simulated a lecture room in which the prerecorded video lectures could be attended and hands-on tutorial rooms in which tutors helped the participants with problems arising when working on the different tutorial exercises. To ensure a good workshop experience these were provided in a controlled JupyterLab environment within a Docker image.

Placing the video lectures on a video platform allowed the participants to deviate from this default setting and watch the lectures at the most convenient time for them. Questions on the lectures and general questions on the hands-on tutorials were answered in several Q&A sessions throughout the days to cover all relevant time zones. For the hands-on tutorials the participants had the option to either attend a morning or an evening session or work on the tutorial independently.

Placing several discussion spots and a separate poster room in the Gather.Town environment promoted communication between the participants, and between the participants and the tutors and lecturers in dedicated poster sessions, and in breaks between different sessions of the workshop.

The format of the workshop was very well perceived and an overwhelming majority of the participants supported the perspective of having more FLEUR workshops like this in the future.

LECTURES **PROGRAM** **TUTORIALS** **TRAINING MATERIAL**



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AiiDA virtual tutorial 2021

5th - 9th July 2021

This year's edition of the AiiDA tutorial took place on 5th-9th July 2021.

The goal of this 5 day-tutorial was to help students and researchers from the field of computational materials science get started with running and writing reproducible workflows. They were introduced by experts in the field (including the developers of the code) to the use of AiiDA, a state-of-the-art framework for provenance tracking and workflow management designed to support high-throughput research. AiiDA already has support for over 50 materials science codes, including established density-functional theory codes such as Quantum ESPRESSO, which was used for this tutorial.

Talk were pre-recorded and made available to participants before the event. Hands-on sessions were held via Zoom, with participants running the tutorial in their browser by accessing a JupyterHub deployment of AiiDAlab. A poster session to which participants were encouraged to participate to present their work was organised.
Computational scientists from both academia and industry were encouraged to apply. Experience with Python was required, but prior experience with AiiDA was not necessary.

Organizers: Marnik Bercx (EPFL), Francisco Fernando Ramirez (EPFL), Giovanni Pizzi (EPFL), Elsa Passaro (EPFL), Andrius Merkys (Vilnius University), Saulius Gražulis (Vilnius University Life Science Center Institute of Biotechnology)

There was no registration fee.

More details in the MAX news

In collaboration with:

Additional links

AiiDA and MAX
AiiDA Official Page

Report

This year's edition of the AiiDA tutorial was once again organized in an entirely virtual format, on 5th-9th July 2021. In order to allow researchers from different time zones to participate, two time slots were organised for each hands-on session. The school had around 100 active participants from 30 different nationalities distributed over 20 time zones. All presentations were pre-recorded and published on the Materials Cloud YouTube channel before the start of the tutorial. The hands-on sessions were organized via Zoom meetings, with the instructors on hand to provide feedback to the participants and breakout rooms made available for one-on-one assistance. At any time during the tutorial week, participants could ask questions on the dedicated Slack workspace.

This year it was decided to introduce two new tools. First, the gather.town platform was used to organise a virtual social event, as well as a mini hackathon on the final day of the tutorial. Second, an AiiDAlab JupyterHub kubernetes cluster was deployed to provide the participants with a uniform and easily accessible work environment. Participants were very happy with the format and tutorial material, and over 88% of them said that they would very likely recommend this tutorial to a colleague.

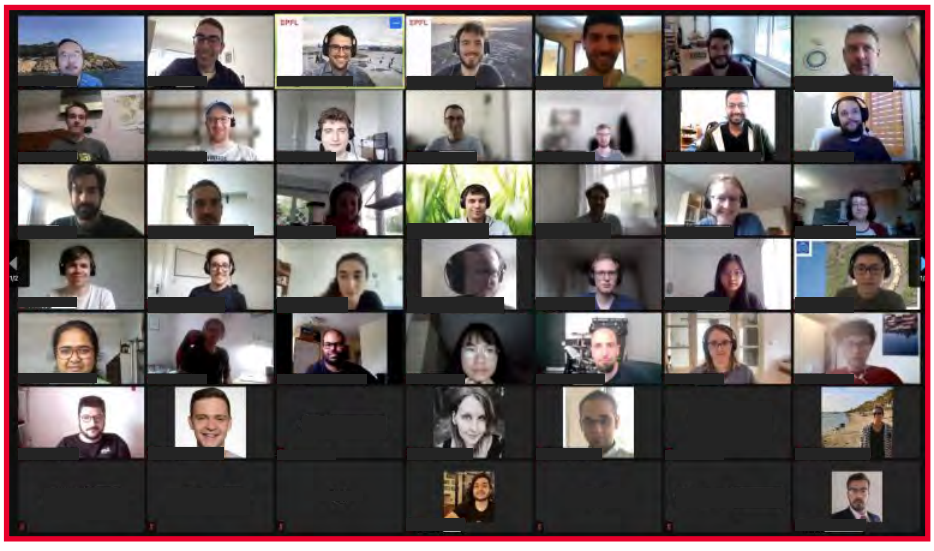
LECTURES **MATERIAL**

More on past training events

2020 School

MAX news

LECTURES



EPFL

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Optimizing Digital Teaching and Communication

September 2021

In September 2021 a hands-on workshop on e-learning techniques and strategies was held, aimed at teachers and researchers in electronic structure and HPC in general. In this new world after the pandemic, experience and needs of those preparing online teaching have evolved. Therefore, the idea of organizing a hands-on workshop on online and blended teaching to address the needs of the post-Covid era came up. There are plenty of reasons to keep elements of teaching in an online form permanently. Some of the workshop's objectives were:

How can the community learn from the past year? How can the community offer the online and blended teaching in a way that leads to better learning and increased student satisfaction? What are the pitfalls that must be avoided?
The challenge of the organizers was to bring this information to the participants in an online format that kept them engaged and motivated.

The participants left the workshop with a set of online teaching materials they had prepared, for their own courses, talks or science communication events. They couldn't hide anonymously behind their laptop, and learnt tricks to avoid the same for their students or their audience.

Organizers: Stefaan Cottenier (Ghent University), Andrea Cucca (CNRS), Rex Godby (University of York), Myrta Grüning (Queen's University Belfast), Gian-Marco Rignanese (Université Catholique de Louvain), Francesco Sottile (Ecole Polytechnique), Matthieu Verstraete (University of Liege), Zeila Zanolli (Utrecht University).

There was no registration fee.

More details in the MAX news

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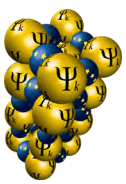

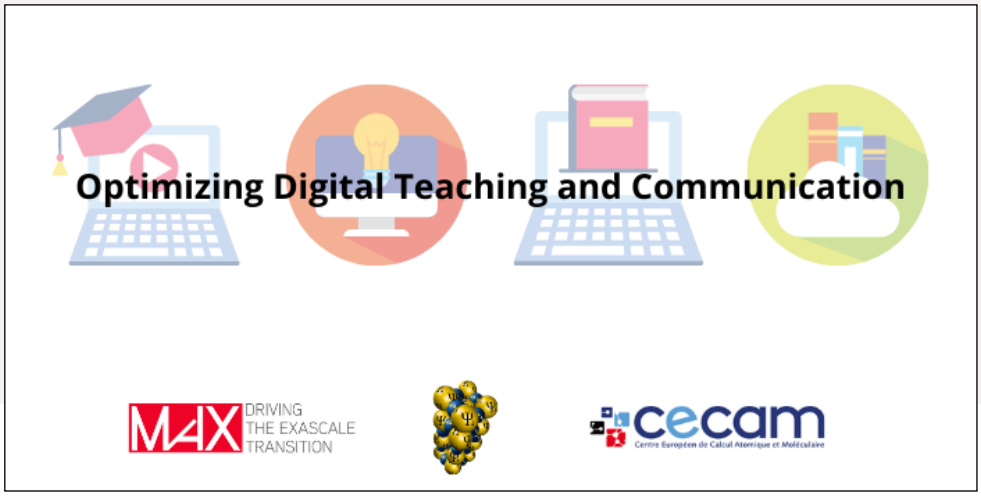

Report

This school had as a goal to demonstrate and practice the new possibilities offered by online teaching, and was organized by scientists for scientists. It was designed in a teach-as-we-preach way: all good online teaching practices that are taught in this school, were used in the school format itself. The school was a three-stage experience.

Stage 1: Potential participants were directed to an online preparation course, where they worked their way through the basic principles and tools for online teaching (including installing some software and making their first hands-on exercises). 16 participants (out of 46 registered people) eventually completed the preparation course and received an entry ticket for stage 2. This selected audience created a subset that was highly motivated and willing to invest time and effort.

Stage 2: During 4 online live sessions (total 16 hours) various aspects of online teaching were explored and demonstrated. Invited lecturers presented their experiences as case-studies. Participants shared their experience with each other in a structured way. Homework tasks were given after every session, and the participants made this homework in teams of 3 people each.

Stage 3: After the 4th live session, there was a 10-day break during which the participants used their new knowledge to create an online learning path for a topic that was relevant for their own teaching. During a concluding 5th live session, these educational paths were peer-reviewed and everyone got a structured written feedback report on their work.

Stage 3-bis: The online preparation course and the material collected during the live sessions will be transformed into a self-paced online course that will be permanently available, for further use by our community.

In conclusion: This was an intense learning experience for a diverse and geographically spread set of participants, made possible by using the power of online teaching tools and concepts -- the very same tools and concepts that were the subject of this school.

COURSE

UNIVERSITEIT GENT

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MAX DRIVING THE EXASCALE TRANSITION

Global numbers on MAX training

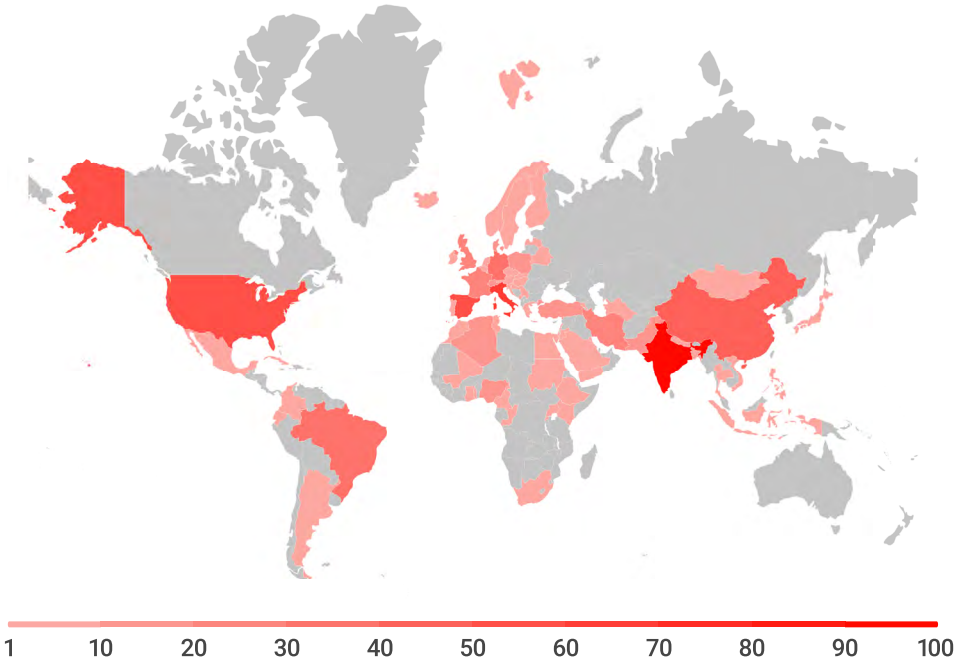
8 Online Events

825 Participants

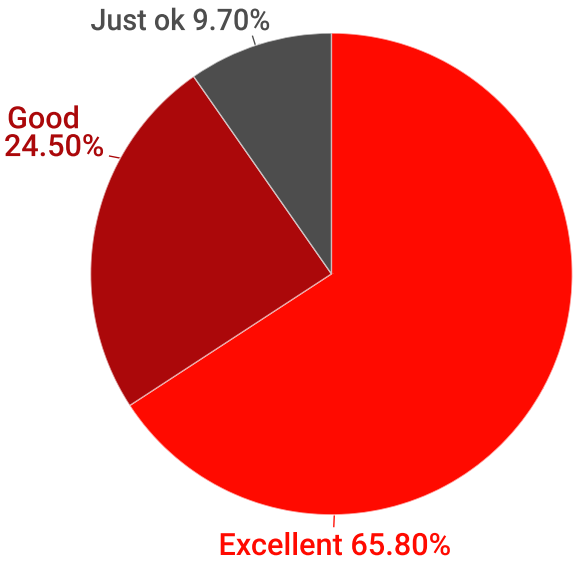
345 Lecture hours

121 Tutors

96 Lecturers

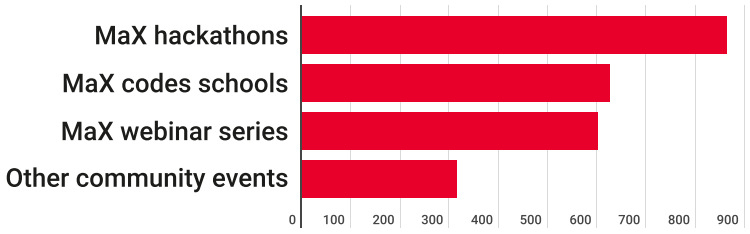


Users' satisfaction



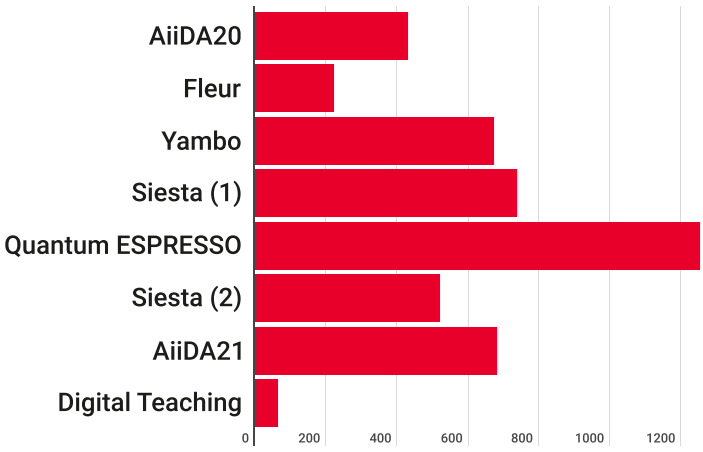
Participants in online MAX Flagship code schools

4570 In person days



Participants in in-person MaX events

2400 In person days



MAX training offer

The strategy of MAX training includes, beside workshops, schools, hackathons, and the presented online events, the following actions:

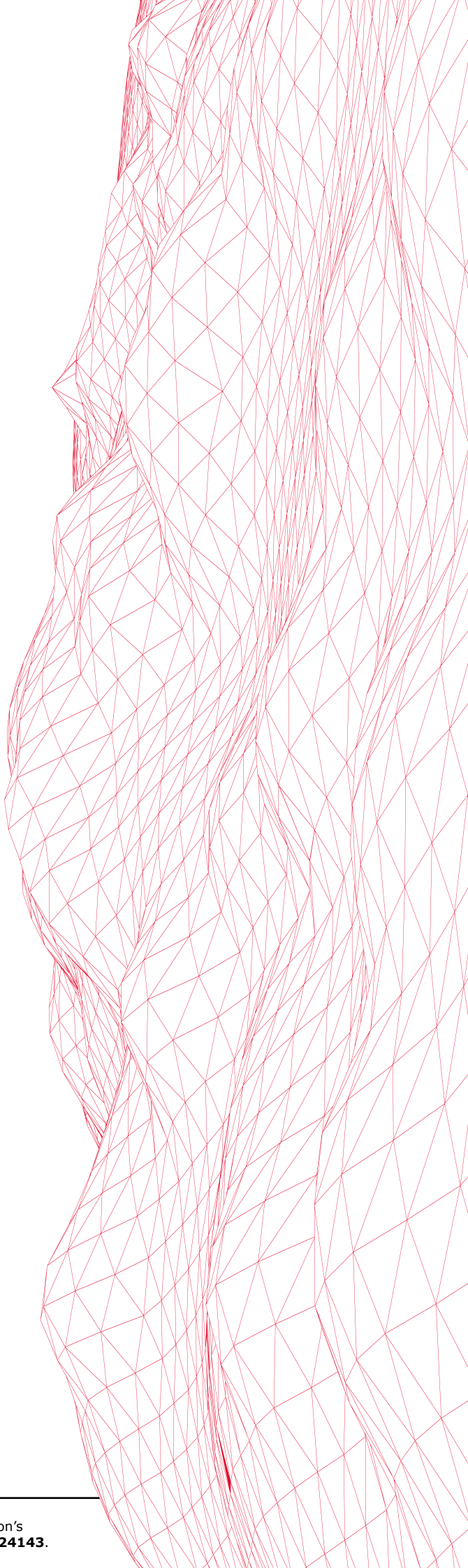
Teaching modules in University - In the MAX training plan, a significant part is given by courses and seminars provided to undergraduate Master students and PhD students as well as University teachers, who wish to learn the use of frontier computational methods within their domain. In order to do so,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

- Hands-on course "Computational Laboratory of Quantum Mechanics" at University of Modena and Reggio Emilia, Italy
- Master in HPC (MHPC) at SISSA/ICTP, Trieste, Italy
- Contribution in the RWTH Aachen University Master Programme, Aachen, Germany
- Course on Atomistic and Quantum Simulation of Materials at EPFL, Lausanne, Switzerland

Training through research - Another successful channel of training is provided directly by hosting researchers in the CoE labs with a one-on-one format, for scientific projects involving the use of MAX flagship codes. Such an instrument is very powerful as it can reach both industrial researchers and academic researchers/ PhD students. In these years, several young researchers were hosted in MAX Labs. The aim is to introduce students and young researchers to the functionalities of the MAX flagship codes and to 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. To participate in this training activity, students and researchers may benefit from the synergy of MAX with the HPC-Europa3 programme.

Training on demand for industry - MAX develops personalised consultancy to industries for specific and targeted needs. The MAX expert team evaluates the request and proposes the best path to follow. Training on demand is included: while MAX training events are usually available free of charge, industrial partners may request dedicated training, with custom topics and calendar (both on and off their premises).

This is MAX consortium



MAX DRIVING THE EXASCALE TRANSITION

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MAX - Materials design at the Exascale has received funding from the European Union's Horizon 2020 - Research and Innovation program - under **Grant Agreement No. 824143**.