HORIZON2020 European Centre of Excellence
Grant Agreement n. 824143

D8.3

Second report on Training and Education

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Due date of deliverable: 30/09/2022

Actual submission date: 18/10/2022

Final version: 10/10/2022

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) /30/09/2022 (month 46)
Website:	www.max-centre.eu
Deliverable No.:	D8.3

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To be cited as: D. Varsano et al., (2022): Second report on Training and Education. Deliverable D8.3 of the H2020 project MAX (final version as of 10/10/2022). EC grant agreement no: 824143, CNR, Modena, Italy.

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D8.3 Second report on Training and Education

Content

Executive Summary

Deliverable 8.3 reports on the education and training activities organised by MAX during the period 01/06/2020-30/09/2022, including data on user participation and involvement. In D8.1 we proposed our structured Training and Education plan, offering a domain-specific program at pan-European level aimed at fostering a new generation of both developers and code users. In D8.2 we reported about the activities carried out in the first 18 months. Here, we report about the last 28 months (M19-M46). During this period, some of the events planned in the first 18 months that had to be postponed due to the COVID-19 outbreak were carried out, reshaped with on-line formats.

This plan is being effectively implemented through different actions, which included:

- Organisation of 11 schools (plus 3 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.
- Organisation of 5 Hackathons and workshops (plus 1 already planned for the near future) devoted to the training of a new generation of code developers.
- MAX contributed to 9 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 numerous researchers in its labs, providing both basic and specialised training on MAX codes and libraries.
- MAX actively contributed to schools and training events organised by other institutions.

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

Due to the COVID-19 outbreak, most of the schools were organised fully on-line due to pandemic constraints, while starting from April 2022 we were able to organise three schools in hybrid format. On-line events were organised according to the strategy conceived during the first months of the COVID-19 outbreak, described in D8.2.

Moreover, MAX contributed to several on-line webinars to ensure its audience proper training during the lockdown.

In order to disseminate and valorize the great amount of training materials collected during this period, MAX together with other institutions has started to develop a web-based archive for the training and dissemination material for simulations and materials modelling.

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

1. Introduction

In the months 19-46, MAX CoE continued the training effort done in the first 18 months, as testified by the organisation of numerous education and training activities, addressing both developers and users. The training activity focused on basic and advanced usage of the MAX flagship codes, with an emphasis on best practice and efficient use of the codes in (pre-)exascale machines, libraries development, workflow implementations, and porting of the code in hybrid architectures.

The training strategy was defined in the first deliverable D8.1 "Training and education programme" that comprises different actions towards different end-users and that can be summarised as follows:

- **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 more expert and the new developers working together on a particular technological aspect of the codes;
- **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.
- **Training on demand**: occasionally, MAX members can organise tailor-made training activities if requested by institutions or projects interested in the flagship codes or some of their features.

The partners involved in WP8 are CNR, SISSA, ICN2, CEA, EPFL, Juelich, ICTP, UGE, in collaboration with the CECAM and Psi-k organisations (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 centres, National Competence Centres).

Most of the events carried out in the M19-M46 period were held in online format, including the ones that were planned for the first period of the CoE postponed for the COVID-19 outbreak. Starting from May 2022 there has been the possibility of carrying out a limited number of events in presence, albeit with some constraints on the number of people and limitations regarding travel due to the restrictions measures still in place in some countries. These events were carried out in hybrid form, thus exploiting the possibility of reaching a greater number of users interested in the MAX training offer, who would have been unable to participate in presence due to the aforementioned limitations. Regarding both fully online and hybrid events, MAX has nevertheless maintained its original plan of providing hands-on sessions by leveraging the experience gained during the first months of the pandemic using teleconferencing platforms that include the use of breakout rooms and exploiting cloud technologies as summarised in Sec. 5 of the previous deliverable D8.2.

In the following, a description of the schools and workshops and the hackathons organised by MAX is presented, following the separation depicted in Table 1. 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. The events highlighted in green have already been organised by MAX and will be held in the near future.

Next, relevant activities belonging to the T8.3 task centred on the coordination and contributions to transversal training initiatives promoted by HPC centres, PRACE and Competence Centres and events coordinated by the CSA are also summarised, as well as teaching modules in Universities targeting Master and PhD students.

Training for MAX flagship codes' users		
AiiDA virtual tutorial Week 2020	07-10/07/2020	
Virtual school on electronic excitations in solids and nanostructures using the Yambo code	8-9 + 15-16/04/2021	
All-electron DFT with Fleur - A Hands-on Tutorial	12-16/04/2021	
Advanced school on Quantum Transport using SIESTA	planned date 23-27/03/2020	actual date 17-21/05/2021

MaX school on Advanced Materials and Molecular Modelling with Quantum ESPRESSO	17-28/05/2021	
First-principles simulations of materials with SIESTA	planned date 2020-05-04/8	actual date 28/06-2/07/2021
On-line tutorial on running and writing workflows with AiiDA	5-9/07/2021	
Ab-initio Many-Body Methods and Simulations with the Yambo Code	4-8/04/2022	
Young Researcher's Workshop on Machine Learning for Materials, 2022	9-13/05/2022	
Wannier Summer School 2022	16-20/05/2022	
Picking Flowers: on-line hands-on tutorial	20-29/09/2022	
Advanced Quantum ESPRESSO tutorial: Hubbard and Koopmans functionals from linear response	9-11/11/2022	
AiiDA online demo and virtual tutorial 2022	4-7/10/2022	
Efficient materials modelling on HPC with Quantum ESPRESSO, Yambo and BigDFT	14-17/11/2022	
Hackathons and workshops for code developers		
Yambo virtual developer's meeting	4-11-18 /12/2020	
Quantum ESPRESSO (QE) virtual hackathon	15-22-29/01/2021	
ESL Workshop 2021	Fall 2020	11-22/10/2021
AiiDA Coding Week 2021	06-10/12/2021	

Hackathon Porting MAX flagship codes on AMD accelerated architectures	27/01-20/02/2022
Co-Design for HPC in Computational Materials and Molecular Science	3-5/10/2022
Visualisation and digital learning schools	
Optimizing Digital Teaching and Communication	15/09/2021-01/10/2021

Table 1: MAX training activities.

The events organized during the reporting period that will be held in the near future are indicated in green.

2. Training events

In the following paragraph, a description of the schools and workshops and the hackathons organised by MAX in the period 01/06/2020-30/09/2022 is available. The events are presented following the list depicted in Table 1.

As in D8.2, the training 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, centred on the coordination and contributions to transversal training initiatives promoted by HPC centres and PRACE and events coordinated by the CSA.

2.1 Training for MAX flagship codes users

1. AiiDA virtual tutorial Week 2020
2. Virtual school on electronic excitations in solids and nanostructures using the Yambo code
3. All-electron DFT with Fleur - A Hands-on Tutorial
4. Advanced School on Quantum Transport using Siesta

5. MAX school on Advanced Materials and Molecular Modelling with Quantum ESPRESSO
6. Siesta: School on First-principles simulations of materials
7. Online tutorial on running and writing workflows with AiiDA
8. Ab-initio Many-Body Methods and Simulations with the Yambo Code
9. Young Researcher's Workshop on Machine Learning for Materials
10. Wannier Summer School 2022
11. Picking Flowers: online hands-on tutorial
12. Aiida online demo and virtual tutorial 2022
13. Advanced Quantum ESPRESSO tutorial: Hubbard and Koopmans functionals from linear response
14. Efficient materials modelling on HPC with Quantum ESPRESSO, Yambo and BigDFTJoint

1. AiiDA virtual tutorial Week, 2020

Venue and date: online from July 7 to July 10, 2020

Organisers: Chris Sewell (EPFL), Marnik Bercx (EPFL), and Giovanni Pizzi (EPFL).

Speakers/Tutors: Sebastiaan Huber, Leopold Talirz, Yakutovich Aliaksandr, Casper Andersen and Francisco Ramirez (EPFL).

Topics: The goal of this 4-day tutorial was to help students and researchers from the field of computational materials science get started with writing reproducible workflows. They have been 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, and they gained in-depth hands-on experience using a tool that they can directly apply to their own research.

The talks were pre-recorded and made available to participants before the event, and hands-on tutorials were held via Zoom. The event focused on in-depth tutorials on the usage of AiiDA and the writing of workflows. It also included some talks on how AiiDA had already been used in production given by the workflow organisers and core developers; on advanced

aspects of workflow management; on designing and writing new AiiDA plugins; and on research data management (RDM) and how to write data management plans (DMPs), especially when using AiiDA and the Materials Cloud.

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

N of participants: 85

Overall assessment: Though incorporating a wide range of time zones presented an interesting challenge, it was decided to split participants into two groups, running duplicate hands-on sessions for each group at different times of the day. All in all, the first virtual AiiDA tutorial was a great success. According to the anonymous feedback questionnaire distributed after the event, participants were very happy with the format and tutorial material, and close to 80% said that more virtual tutorials should be organised in the future, even once travelling no longer is an issue. Many valuable suggestions were received, to be taken into consideration to further improve the next tutorials. A detailed report is available here.

Website: http://www.max-centre.eu/news-events/aiida-virtual-tutorial
https://www.aiida.net/aiida-virtual-tutorial-july-2020/

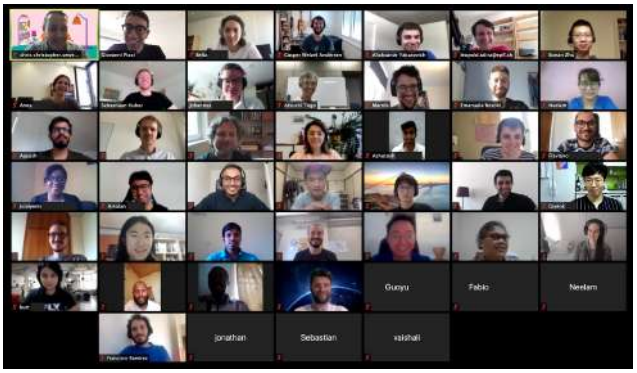

Fig 1. Group picture of the AiiDA virtual tutorial Week 2020.

2. Virtual school on electronic excitations in solids and nanostructures using the Yambo code

Fig 2. Promotional banner of the virtual school on

electronic excitations in solids and nanostructures using the Yambo code

Venue and date: online on April 8-9 and 15-16, 2021.

Organisers: Myrta Grüning (Queen's University Belfast), Conor Hogan (CNR ISM), Maurizia Palummo (University of Rome Tor Vergata), Daniele Varsano (CNR Nano).

Speakers and Tutors: Daniele Varsano (CNR Nano), Michele Re Fiorentin (Politecnico Torino), Fulvio Paleari (CNR ISM), Myrta Grüning (Queen's University), Claudio Attaccalite (CNRS), Margherita Marsili (UniBo), Dario A. Leon Valido (CNR Nano), Andrea Ferretti (CNR Nano), Samaneh Ataei (CNR Nano), Alberto Guandalini (CNR Nano), Davide Sangalli (CNR ISM), Marco D'Alessandro, Conor Hogan (UniRoma2), Andrea Marini (CNR ISM), Nicola Spallanzani (CNR Nano), Maurizia Palummo (UniRoma2), Pedro Melo (CNR ISM), Elena Molteni (UniMI), Miki Bonacci (CNR Nano), Matteo Zanfrognini (CNR Nano), Ignacio Alliati (Queen's University), Daniel Murphy (Queen's University), Pino D'Amico (CNR Nano), Claudia Cardoso (CNR Nano), Ivan Marri (CNR Nano & Unimore), Ridwan Agbaoye (CNR Nano), Bo Peng (University of Cambridge).

Topics: The school introduced the participants to MBPT approaches and to the demonstration of ab-initio MBPT simulations using the Yambo code. The covered topics ranged from basic lectures on general MBPT concepts to more specific approximations and implementations for applications in materials science. General topics included the diagrammatic approach, Hedin equations, self-energy and quasiparticles, the GW approximation, linear response, and the Bethe-Salpeter equation. Strong focus was given on the connection with experimental observables (photoemission, absorption, photoluminescence). Besides theoretical lectures, the participants were guided to hands-on sessions, where they learned to set up calculations using the Yambo code, to converge the main parameters in order to obtain meaningful results, and to post-process the results so as to have a comprehensive data analysis and visualisation of the results.

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

N of participants: 159

Overall assessment: This was the first Yambo school performed completely online due to the pandemic outbreak. The school was organised using the zoom platform, and theoretical lectures were recorded and made publicly available in the Yambo and MAX YouTube channels on a daily basis. The hands-on sessions were organised by dividing the students in Zoom breakout rooms in a group of 6/8 students per tutor. Multiple options were given for the usage of the code, ranging from direct installation, to Quantum Mobile virtual machine and docker container. The feedback received from the participants has been extremely positive, both theoretical sessions and hands-on were positively evaluated, as well as the skill and responsiveness of lecturers and tutors. Overall score from anonymous feedback questionnaires was 4.7/5.

Website: https://www.cecam.org/workshop-details/1081#program-1081

Fig 3. Group picture of the virtual school on

electronic excitations in solids and nanostructures using the Yambo code

3. All-electron DFT with Fleur - A Hands-on Tutorial

Venue and date: online from April 12 to, April 16 2021 + extra Q&As session on April 22 and April 29

Organisers: Daniel Wortmann, Uliana Alekseeva, Gregor Michalicek (Jülich).

Speakers: Stefan Blügel, Daniel Wortmann, Gregor Michalicek, Alexander Neukirchen, Robin Hilgers, Gustav Bihlmayer, Dongwook Go, Stefan Rost, Uliana Alekseeva, Francisco Fernando

Ramirez, Jens Bröder, Vasily Tseplyaev, Christoph Friedrich, Dmitrii Nabok, Matthias Redies, Henning Janssen.

Topics: 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 focused on training the participants in using our all-electron FLAPW DFT code FLEUR. A special attention was paid to the usage of FLEUR within the AiiDA infrastructure to build automatic workflows applicable to materials screening applications.

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

N of participants: 44 (n. of applicants: 155)

Overall assessment: Placing several discussion spots and a separate poster room in the Gather.Town environment promoted communication among 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 (overall score from anonymous feedback questionnaire 4.3/5), and an overwhelming majority of the participants supported the perspective of having more FLEUR workshops like this in the future. All the lectures were recorded and made available in the MAX YouTube channel.

Website: http://www.max-centre.eu/news-events/all-electron-dft-fleur-hands-tutorial
https://www.flapw.de/MaX-5.0/handson/

Fig 4. Introductory slide of the talk by Stefan Bluegel on "DFT - A brief reminder of what you know already" @ All-electron DFT with Fleur - A Hands-on Tutorial 2021

4. Advanced school on Quantum Transport using SIESTA

Venue and date: online from May 17 to 21, 2021

Organisers: Simona Achilli (University of Milan), Mads Brandbyge (Technical University of Denmark), Thomas Frederiksen (DIPC - Donostia International Physics Center), Pablo Ordejón (ICN2), Nick Papior (Technical University of Denmark), Zeila Zanolli (Utrecht University).

Speakers: Gaetano Calogero (CNR), Thomas Frederiksen (DIPC), P. Khomyakov (Synopsis), Pablo Ordejón (ICN2), Nick Papior (Technical University of Denmark), Sofia Sanz, (DIPC), Zeila Zanolli (Utrecht University).

Topics: 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 introduced novel methods used for materials research modelling, the advanced features of SIESTA code, such as the calculations of non-equilibrium properties using the TranSIESTA/TBtrans approach and the python framework SISL.

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

N of participants: 119

Overall assessment: The participants highly appreciated the organisation of the school, the lectures and the hands-on sessions. Also, the used online tools for discussion (discord forum) was positively evaluated. Some suggestions on how to improve the format were collected.

Overall score from anonymous feedback questionnaire: 4.4/5. All the lectures were recorded and made available in the MaX YouTube channel.

Website: https://www.cecam.org/workshop-details/4

Fig 5. Pablo Ordejón on "TranSIESTA for Electrochemistry" @ Advanced school on Quantum Transport using SIESTA 2021

5. MaX school on Advanced Materials and Molecular Modelling with Quantum ESPRESSO

Venue and date: online from May 17 to 28, 2021

Organisers: Stefano Baroni (SISSA), Ralph Gebauer (ICTP), Anton Kokalj (Jožef Stefan Institute), Wei Ren (Shanghai University), Alessandro Stroppa (CNR-SPIN), Ivan Girotto (ICTP), Ivan Carnimeo (SISSA).

Speakers: Alessandro Stroppa (CNR-SPIN), Andrea Urru (ETHZ), Iurii Timrov (EPFL), Anton Kokalj (Jozef Stefan Institute), Ari Paavo Seitsonen (École Normale Supérieure), Elisa Molinari (CNR Nano), Francesco Mauri (Sapienza University of Rome), Ivan Carnimeo (SISSA), Marnik Bercx (EPFL), Nicola Spaldin (ETH Zurich), Oscar Baseggio (SISSA), Paolo Giannozzi (University of Udine), Pietro Bonfà (University of Parma), Pietro Delugas (SISSA), Ralph Gebauer (ICTP), Riccardo Bertossa (SISSA), Roberto Car (Princeton University), Sandro Scandolo (ICTP), Stefan Bluegel (Peter Grünberg Institut and Institute for Advanced Simulation), Stefano Baroni (SISSA), Stefano De Girongoli (SISSA), Xingao Gong (Fudan University).

Topics: 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). 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.

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

N of participants: 120 for organisational reasons (1292 applicants).

Overall assessment: All participants expressed their enthusiasm and gratitude for the organisation of the online school. The event was, for the first-time, entirely held online, with an innovative two-weeks 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 is now available on the web.

Website: https://indico.ictp.it/event/9616/
http://www.max-centre.eu/news-events/max-school-advanced-materials-and-molecular-modelling-quantum-espresso

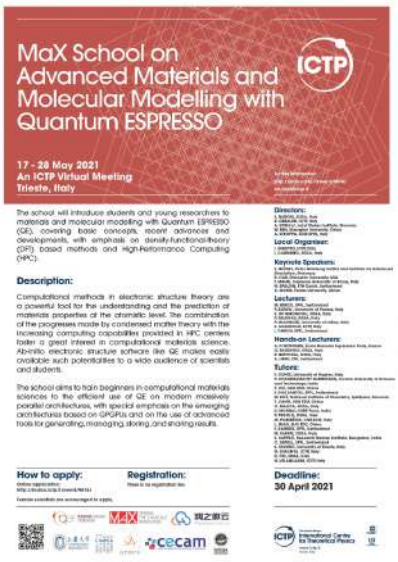

Fig 6. Poster of the MaX school on Advanced Materials and Molecular Modelling with Quantum ESPRESSO

A detailed report is available here.

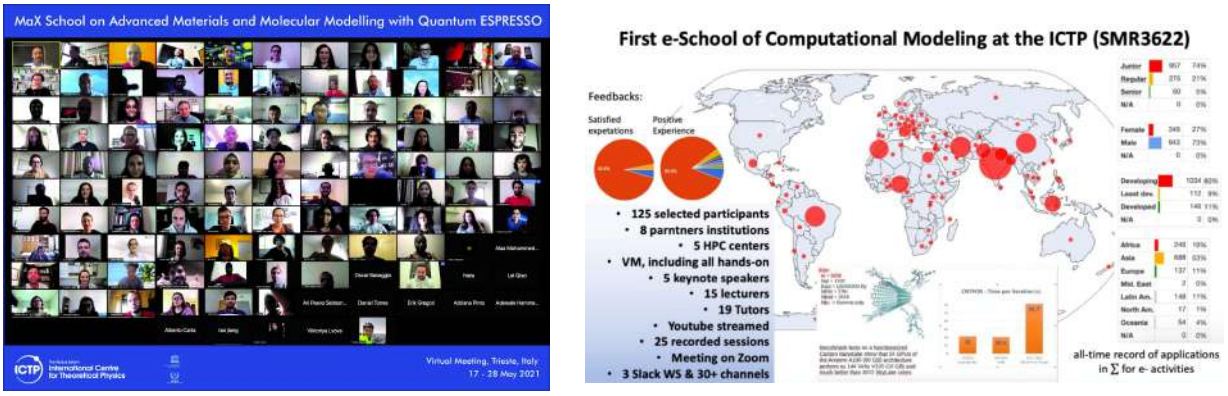

Fig 7. Group picture of the MaX school on Advanced Materials and Molecular Modelling with Quantum ESPRESSO (on the left) and statistics about the school participants (on the right)

6. First-principles simulations of materials with SIESTA

Venue and date: online from June 28 to July 2, 2021.

Organisers: Emanuele Bosoni (ICMAB-CSIC), Antonio Cammarata (Czech Technical University In Prague), José María Escartín Esteban (ICN2), Alberto Garcia (ICMAB-CSIC), Pablo Ordejon (ICN2), Miguel Pruneda ((ICN2), Zeila Zanolli (Utrecht University).

Speakers: Bogdan Guster (Institute of Condensed Matter and Nanosciences, UCLouvain), Eduardo Cisternas (Universidad de La Frontera), Jose Angel Silva-Guillén (Fundación IMDEA Nanociencia), Andrei Postnikov (University of Lorraine, LCP-A2MC), Simona Achilli (University of Milan), Arsalan Akhtar (ICN2), Emanuele Bosoni (ICMAB-CSIC), Ernane De Freitas Martins (ICN2), Vladimir Dikan (ICMAB-CSIC), Roberta Farris (ICN2), Pol Febrer Calabozo (ICN2), Sara G Mayo (Universidad Autónoma de Madrid), Alberto Garcia (ICMAB-CSIC), Xu He (ICN2), Dilson Juan (University of Cantabria), Javier Junquera (Universidad de Cantabria), Pablo Ordejón (ICN2), Federico Nicolás Pedron (ICN2), Jorge Pilo (ICN2), Yann Pouillon (Simune Atomistics), Miguel Pruneda (ICN2), Roberto Robles (CFM/MPC, CSIC-UPV/EHU), Jose M. Soler (Autonomous University of Madrid), Nils Wittemeier (ICN2), Emilio Artacho (University of Cambridge), Ramón Cuadrado Del Burgo (University of Southampton).

Topics: The school was addressed to students and researchers from different disciplines who already used, or planned to use, first-principles techniques to simulate properties of matter at the atomic scale. In particular, the school focused on the SIESTA method, and allowed participants to learn its essential theoretical foundations, and to use the SIESTA code effectively. Pre- and post-processing tools were also presented.

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

N of participants: 135 (263 applicants)

Overall assessment: 4.64 stars on a scale from 1 to 5 stars. Only 7% of the respondents rated the school with less than 4 stars, while 79% of the respondents awarded the top rating. Two thirds of the respondents considered that their SIESTA skills qualitatively improved during the school.

It is relevant to notice that, in addition, about a fifth of the respondents reported that their SIESTA skills qualitatively improved in the 2.5 months after the end of the school. This suggests that the school triggered further learning during that period.

*Web*site: https://www.cecam.org/workshop-details/5

Fig 8. Miguel Pruneda on "Time-dependent DFT in real time" @ First-principles simulations of materials with SIESTA school 2021

7. Online tutorial on running and writing workflows with AiiDA

Venue and date: online from July 5 to 9, 2021.

Organisers: Francisco Ramirez (EPFL), Marnik Bercx (EPFL), and Giovanni Pizzi (EPFL), Andrius Merkys (Vilnius University), Saulius Gražulis (Vilnius University)

Speakers: Leopold Talirz, Sudarshan Vijay, Aliaksandr Yakutovich, Casper Andersen, Flaviano dos Santos, Carl Simon Adorf and Chris Sewell (all from EPFL).

Topics: The goal of this 5-day tutorial was to help students and researchers from the field of computational materials science to 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.

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

N of participants: 136

Overall assessment: The tutorial was completely held online, and new technologies to support teaching efforts were adopted. The Zoom platform was used to handle the Q&As, hand-on sessions and one-on-one assistance. Slack was also used before to handle general questions and support. In this edition, two new tools were adopted: besides the use of the gather.town platform, an AiiDAlab JupyterHub cluster was set up and deployed to provide the participants with a uniform and accessible work environment. The feedback on these technological aspects was positive. All in all, the virtual AiiDA tutorial was a great success, the participants were very happy with the format and tutorial material, and over 88% said that they would be very likely (8 or more out of 10) to recommend this tutorial to a colleague. Many valuable suggestions to be considered to further improve the next tutorials were received.

A detailed report is available here.

Website: https://www.aiida.net/aiida-virtual-tutorial-july-2021/
http://www.max-centre.eu/news-events/introduction-running-reproducible-workflows-aiida

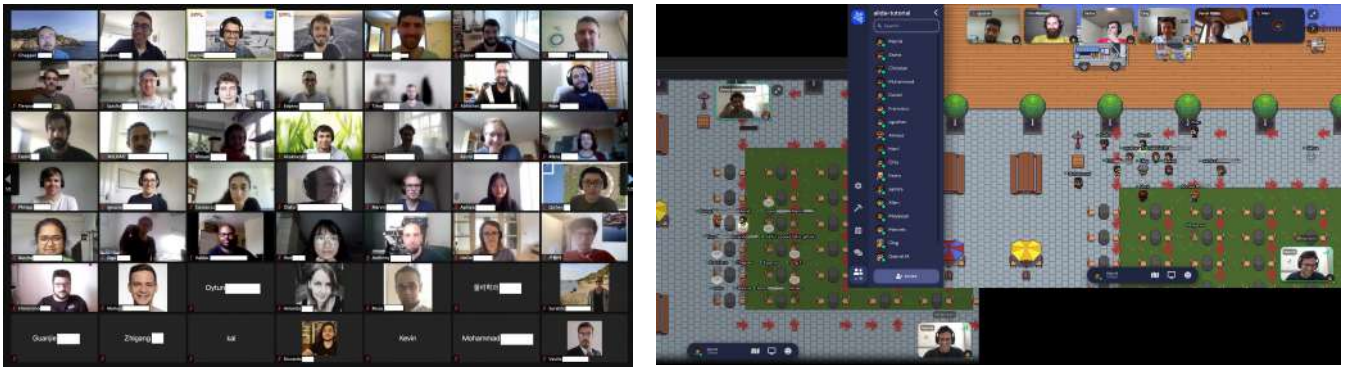

Fig 9. Group picture of the Online tutorial on running and writing workflows with AiiDA (on the left) and a screenshot of the gather.town social event in which a session of scientific speed dating was proposed

8. Ab-initio Many-Body Methods and Simulations with the Yambo Code

*Venue and date: h*ybrid, online and at ICTP Kastler Lecture Hall, Trieste (IT), from April 4 to 8, 2022.

Organisers: Claudio Attaccalite (CNRS, Aix-Marseille University), Andrea Marini (CNR-ISM), Maurizia Palummo (Università di Roma Tor Vergata), Davide Sangalli (CNR-ISM), Daniele Varsano (CNR-NANO), Nicola Seriani (ICTP).

Speakers: Alberto Guandalini (CNR-NANO), Andrea Marini (CNR-ISM), Daniele Varsano (CNR-NANO), Bartomeu Monserrat (University of Cambridge), Dario Alejandro Leon Valido (CNR-NANO), Claudio Attaccalite (CNRS, Aix-Marseille University), Davide Sangalli (CNR-ISM), Elena Cannuccia (Aix-Marseille University), Fulvio Paleari (CNR-NANO), Alejandro Molina-Sanchez (University of Valencia), Matteo Gatti (CNRS École Polytechnique), Nicola Seriani (ICTP), Pedro Melo (University of Utrecht), Polina Sheverdyaeva (CNR-ISM), Sivan Refaely-Abramson (Weizmann Institute).

Topics: General topics included self-energy and quasiparticles concepts, the GW approximation, and the Bethe-Salpeter equation, all placed in the context of and linked with experimental measurements (photoemission, absorption, photoluminescence). Both theoretical and technical lectures were offered, as well as dedicated hands-on sessions where students learned to use the code for materials of current research interest and to optimise its use in a parallel environment. Several post-processing tools for the analysis of the results have also been introduced and practically applied.

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

N of participants: 144 (all the details are available here)

Overall assessment: The school was held in hybrid mode: 23 participants attended the school in presence, the remaining 121 online mode. The number of in-person attendance was limited by the capacity of the classroom reduced for the COVID-19 rules. Most of the lectures were conducted in person and broadcasted through the zoom platform. The hands-on were managed by 6 tutors in the flesh, while 18 tutors followed the students remotely in the zoom breakout rooms. In this school, we tested for the first time a seamless cloud environment with graphical interfaces and scientific programs running on multicores high-end computer platforms. The cloud platform was accessible via a web browser that provided a graphical interface to a Linux desktop, avoiding the need of pre-installation of software in the user machines. Given the very positive feedback received on this technological aspect, we plan to use cloud VM in future events. Overall the school was very successful judging from the appreciation received in anonymous feedback form with a global score of 4.7/5.

Website: https://indico.ictp.it/event/9780/
http://www.max-centre.eu/news-events/max-school-ab-initio-many-body-methods-and-simulations-yambo-code

Fig 10. The poster (on the left) and one moment (on the right) of the Ab-initio Many-Body Methods and Simulations with the Yambo Code 2022

9. Young Researcher's Workshop on Machine Learning for Materials 2022

Venue and date: SISSA Miramare Campus Trieste (IT) from May 9 to 13, 2022.

Organisers: Claudio Zeni (SISSA), Kevin Rossi (EPFL), Stefano de Gironcoli (SISSA), Milica Todorović (University of Turku), Patrick Rinke (Aalto University).

Speakers: Francesca Grisoni (Eindhoven University of Technology), Boris Kozinsky (Harvard University), Zachary Ulissi (Carnegie Mellon University), Núria López (Institute of Chemical Research of Catalonia), Matthias Rupp (University of Konstanz), Sašo Džeroski (Jozef Stefan Institute), Alessandro Laio (SISSA), Kristof T. Schütt (Technische Universität Berlin), Julia Westermayr (University of Warwick), Johannes Margraf (Fritz-Haber-Institut der MPG), Lars Banko (Ruhr-Universität Bochum), Felix Andreas Faber (University of Cambridge), Milica Todorović (University of Turku), Aldo Glielmo (Banca d'Italia), Franco Pellegrini (SISSA), Anton Bochkarev (Ruhr-Universität Bochum), Rianne van den Berg (Microsoft Research), Andrea Anelli (Roche), Robin Winter (Bayer), Sebastiano Saccani (Aindo).

Topics: the workshop's objective was to cultivate the ground for the next generation of scientists who will be able to proactively and efficiently exploit data-driven techniques in materials modelling. Bringing together young researchers, experts from computer science and applied mathematics, and renowned scientists in the field of chemistry and physics, the goal was to discuss the present and future of machine learning for materials.

The workshop was free of charge, and consisted of 4-half days of introductory school (Monday to Wednesday), followed by 4-half days of conference (Wednesday to Friday). Participants could choose whether to attend both modules, or only the conference.

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

N of participants: 94 participants in person, 237 participants online.

Overall assessment: The workshop was specifically designed to address the needs for multi-disciplinary cross-contamination, and we received resounding feedback about how such an effort was successful. All (to our knowledge, and according to a survey, overall score 4.6/5) participants to the workshop, be it an invited speaker, an online attendee, a poster presenter, or a young researcher that attended their first conference on the topic, were largely positive about the structure, topics, and organisation of the event. All talks, tutorials, and panel discussions that took place during the workshop were recorded and uploaded on YouTube, and the conference's website, thus making high-quality scientific content available to anyone. The presence of industry representatives (Roche, Bayer, Microsoft Research, AIndo) on one hand offered an overview of possible career pathways for participants. From an alternative perspective, the state-of-the-art methods and achievements obtained by our community were promoted to these R&D teams. A detailed report can be found here.

Website: https://ml4m.xyz/
http://www.max-centre.eu/news-events/young-researchers-workshop-machine-learning-materials-2022

Fig 11. The promotional banner (on the left) and a moment (on the right) of the Young Researcher's Workshop on Machine Learning for Materials 2022

10. Wannier Summer School 2022

Venue and date: ICTP Trieste (IT) and online from May 16 to 20, 2022.

Organisers: Antimo Marrazzo (University of Trieste), Sinisa Coh (University of California, Riverside), Roxana Margine (Binghamton University - State University of New York), Giovanni Pizzi (EPFL), Stepan Tsirkin Sirkin (University of Zurich), Nicola Seriani (ICTP).

Speakers: R. Arita (Tokyo University and RIKEN, Japan), S. Beck (Flatiron Institute, USA), F. Giustino (UT Austin, USA), L. Lin (UC Berkeley, USA), N. Marzari (EPFL, Switzerland), A. Mostofi (Imperial College London, UK), Y. Nomura (Keio University, Japan), S. Poncé (EPL, Belgium), J. Qiao (EPFL, Switzerland), R. Resta (CNR-IOM, Italy), I. Souza (CFM and UPV, Spain), K. Thygesen (DTU, Denmark), D. Vanderbilt (Rutgers University, USA), M. Vergniory (DIPC, Spain), V. Vitale (Imperial College London, UK), Q. Wu (IOPCAS, China), J. Yates (Oxford University, UK).

Topics: This 5-day school consisted of lectures and hands-on sessions on a wide range of electronic-structure methods based on Wannier functions (WFs). The event targeted graduate students, early-career scientists, and experienced users. The school included highlight talks that provided a historical and broad perspective on WFs in electronic structure, a broad set of dedicated lectures to the theory and methods of WFs, as well as hands-on tutorials at basic and advanced levels.

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

N of participants: 95 (half in presence, half in remote, all the details are available here).

Overall assessment: Each participant got access to a dedicated VM instance on the ICTP Cloud for the entire duration of the workshop. The VM was fundamental to ensure that all participants would execute the tutorials on the same software environment. The results from the feedback forms were remarkably good, the event received high scores on all probed aspects. The vast majority of participants would really recommend this school to a colleague: on a scale of 0-10, 83% of the respondents gave a mark of 8/10 or higher, and 43% actually replied with a full 10/10. The school organisation and content were also rated very high, and the respondents confirmed their skills improved thanks to the event. All the lectures were recorded and made available on YouTube. A detailed report can be found here.

Website: https://indico.ictp.it/event/9789/
http://www.max-centre.eu/events/wannier-2022-summer-school

Fig 12. The group picture (on the left) and a moment (on the right) of the Wannier Summer School 2022

11. Picking Flowers: online hands-on tutorial

Venue and date: online from September 20 to September 29, 2022

Organisers: Daniel Wortmann and Gregor Michalicek (FZ Jülich)

Speakers: Stefan Blügel, Daniel Wortmann, Gregor Michalicek, Gustav Bihlmayer, Alexander Neukirchen, Robin Hilgers, Henning Janssen, Dongwook Go, Uliana Alekseeva, Matthias Redies, Francisco Fernando Ramirez, Jens Bröder, Vasily Tseplyaev, Christoph Friedrich, Dmitrii Nabok, Stefan Rost (all from Jülich).

Tutors: Daniel Wortmann, Gregor Michalicek, Gustav Bihlmayer, Alexander Neukirchen, Henning Janssen, Johanna Carbone, Dongwook Go, Christoph Friedrich, Dmitrii Nabok, Jörn Stöhler (all from Jülich).

Topics: This event targeted new and more experienced users of the FLEUR code, who wanted to learn in an interactive manner the usage of the code. It lasted three days a week (from Tuesdays to Thursdays) with a session with talks on FLEUR related topics each day and two (identical) hands-on sessions each day to fit time constraints + Q&A sessions to discuss with developers and presenters.

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

N of participants: 65 active participants (145 registered).

Overall assessment: The workshop was designed for a pure online participation in a Gather.Town setup, with pre-recorded video lectures either accessible in live sessions or

independent of the workshop schedule on a video-sharing platform. To make the workshop accessible to people from many different time zones, hands-on and Q&A sessions were provided twice on each workshop day. For a common software environment, the hands-on sessions were technically realised in terms of Jupyter notebooks within a docker image running on participant's hardware and a backup solution on the mybinder platform. This setup kept the number of technical issues during the workshop very low.

Both, lectures and hands-on sessions, received very positive feedback with respect to all evaluated aspects like understandability, usefulness, and coverage of relevant topics. The average evaluation by the participants was 4.5 / 5.0 points for the lectures and 4.4 / 5.0 points for the hands-on sessions. Registered participants not taking an active part in the workshop most often mentioned time constraints as the reason.

Website: https://www.flapw.de/MaX-6.0/handson/

http://www.max-centre.eu/news-events/picking-flowers-hands-fleur-tutorial

12. Aiida online demo and virtual tutorial 2022 *(event organised during the project timeframe, and held after MAX conclusion)*

Venue and date: Online from October 4 to October 7, 2022

Organisers: Chris Sewell (EPFL), Marnik Bercx (EPFL) and Giovanni Pizzi (EPFL).

Speakers: Chris Sewell (EPFL), Marnik Bercx (EPFL) and Giovanni Pizzi (EPFL), Jusong Yu (EPFL), Francisco Ramirez (EPFL), Sebastiaan Huber (EPFL), Flaviano dos Santos (EPFL), and Carl Simon Adorf (EPFL).

Topics: The goal of this 4 day-tutorial is to help students and researchers from the field of computational materials science get started with running and writing reproducible workflows. They will be introduced by experts in the field (including the developers of the code) to the use of AiiDA, and will 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: 80

Website: https://www.aiida.net/aiida-online-demo-and-virtual-tutorial-2022/

In collaboration with Microsoft Quantum, the AiiDA team (EPFL) worked on providing a template for deploying an AiiDAlab JupyterHub deployment on Microsoft Azure. This is built

based on the AiiDAlab docker stack image also discussed in T7.3. Full instructions on how to set up the infrastructure using Terraform can be found on the GitHub repository[1]. Such a deployment has also been used in this tutorial.

13. Advanced Quantum ESPRESSO tutorial: Hubbard and Koopmans functionals from linear response *(event organised during the project timeframe, it will be held after MAX conclusion)*

Venue and date: online from November 9 to November 11, 2022.

Organisers: Iurii Timrov (EPFL), Nicola Colonna (PSI), Matteo Cococcioni (Univ. Pavia), Andrea Ferretti (CNR Nano).

Speakers: Leoor Kronik (Weizmann Institute of Science), Renata Wentzcovitch (Columbia University), Matteo Gatti (EPFL), Nicola Marzari (EPFL and PSI), Giovanni Pizzi (EPFL and PSI), Edward Linscott (EPFL), Iurii Timrov (EPFL), Nicola Colonna (PSI), Andrea Floris (Lincoln University), Andrea Ferretti (CNR Nano), Matteo Cococcioni (University of Pavia).

Topics: The goal of this tutorial is to introduce PhD students, postdocs, and junior scientists to the use of advanced functionals aimed at modelling complex materials, such as the extended Hubbard and Koopmans functionals. By eliminating self-interaction errors and restoring total energy piecewise linearity, these advances broaden the scope of DFT by either improving the ground-state description of transition-metal and rare-earth compounds or by giving access to accurate spectral properties (like fundamental band gaps and band structures). Indeed, Hubbard and Koopmans functionals are deeply rooted in the theory of DFT and try to address fundamental difficulties of its Kohn-Sham declination. Their actual implementation also takes advantage of linear-response theory through the self-consistent incarnation contained in density-functional perturbation theory (DFPT).

In view of these goals, the first day of the tutorial will be devoted to an introduction to fundamental aspects of DFT using local and semi-local functionals, its application to materials science and physics, and its limitations. In the next 2 days, the tutorial will cover the theoretical framework of Hubbard and Koopmans functionals (the main topic of this event). The reference computational platform of the tutorial will be Quantum ESPRESSO (QE), a widely used open-source electronic-structure software, which implements both extended Hubbard and Koopmans functionals.

The intensive program will offer (i) presentations by keynote speakers with a broad overview on the topic of the day, (ii) theoretical and technical lectures by some of the leading

[1] https://github.com/aiidalab/aiidalab-on-azure

developers of the QE project, as well as (iii) demonstrations and dedicated hands-on sessions on both basic and more advanced features. Importantly, the participants will learn how to compute the Hubbard parameters and Koopmans screening coefficients from DFPT. Since QE is an open-source platform for ab initio calculations, the tutorial will provide a practical and operative knowledge of the discussed topics that participants will be able to use directly in their own research or educational activities.

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

N. of participants: To date (Sept. 30, 2022), more than 850 applications were received and we expect to accept most of the applicants (up to 1000, which is the upper limit imposed by the Zoom webinar app we are going to use.)

Website: https://sites.google.com/view/hubbard-koopmans/home?authuser=0

14. Efficient materials modelling on HPC with Quantum ESPRESSO, Yambo and BigDFT

(event organised during the project timeframe, it will be held after MAX conclusion)

Venue and date: online from November 14 to 17, 2022.

Organisers: Kjartan Thor Wikfeldt (ENCCS - SW), Lilit Axner (ENCCS - SW), Daniele Varsano (CNR Nano - IT), Ivan Carnimeo (SISSA - IT), Laura Ratcliff (Univ. Bristol. - UK)

Speakers: Iurii Timrov (EPFL, Switzerland), Ivan Carnimeo (SISSA, Italy), Pietro Delugas (SISSA, Italy), Stefano Baroni (SISSA, Italy), Daniele Varsano (CNR Nano, Italy), Andrea Ferretti (CNR Nano, Italy), Davide Sangalli (CNR ISM, Italy), Fulvio Paleari (CNR Nano, Italy), Giovanni Pizzi (EPFL and PSI, Switzerland), Laura Ratcliff (Univ Bristol, UK), Martina Stella (ICTP, Italy), Luigi Genovese (CEA, France).

Topics: The 4-day school is an event organised together with EuroCC National Competence Centre, Sweden ENCCS. The event will be entirely online, conceived for academic and industrial users, in which fundamental concepts of molecular modelling on HPC will be given, and some of the most modern codes (Quantum ESPRESSO, Yambo, BigDFT) will be introduced. Best practices for an efficient exploitation of HPC resources will be also discussed, with particular emphasis on how to use the different schemes of data distribution in combination with the different parallelization and acceleration schemes (MPI, OpenMP, GPU-offload) available in these three *MAX* codes. Hands-on sessions will be held using zoom breakout rooms, in which participants will be able to practise and run simulations in an HPC environment using the Vega supercomputer.

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

N. of participants: We expect the participation of 30-50 learners from European countries.

Website: https://enccs.se/events/2022-11-efficient-materials-modelling/

2.2 Hackathons and workshops for code developers

As in the first period, *MAX* continued to (co-)organise Hackathons and workshops for developers, in order to guarantee proper training for the new generations of *developers*. Due to the impossibility to organise in-person meetings in the period of COVID-19 restrictions, we organised online events in order to maintain a close contact between users and leading code developers and experts.

1. Yambo Virtual developer's meeting 2020
2. Quantum ESPRESSO (QE) virtual hackathon 2021
3. ESL Workshop 2021
4. AiiDA Coding Week 2021
5. Hackathon Porting MAX flagship codes on AMD accelerated architectures 2022
6. Co-Design for HPC in Computational Materials and Molecular Science 2022

1. Yambo Developers' meeting: Yambo developer Fridays

Venue and date: online on December 4, 11, and 18, 2020.

Organisers: the Yambo developers team.

Speakers: A. Marini, M. Gruening, M. Bonacci, D. A. Leon Valido, D. Varsano, E. Molteni, C. Attaccalite, D. Sangalli, F. Paleari, N. Spallanzani, A. Ferretti, P. D'Amico, M. Marsili, A. Guandalini, F. Affinito.

Topics: discussion on the status and future programs of the Yambo code, ongoing and future developments, next release, Python platform, extending GPU porting, optimization, best practice, and planning of training events.

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

N of participants: 30

Overall assessment: Despite the fact the event was held completely online due to COVID-19 restrictions, the meeting was an occasion for young developers to present their work on new implementations in the code and discuss technical details with more experienced developers. The program was designed to give space to the younger developers to present their work, reserving time for discussions. Moreover, the young developers had the opportunity to have a more general view of the Yambo project as a whole. Developers keenly discussed the porting of Yambo to GPU machines and the extension of the current CUDA-Fortran porting to additional backends (OpenACC, OpenMP5), important to support in full the EuroHPC pre-exascale machines. Possible developments coming from the user community were also discussed. A detailed report can be found here.

Website: http://www.max-centre.eu/sites/default/files/ydm_program.pdf

Fig 13. Group picture and banner of the Yampo Developers' meeting 2020

2. Quantum ESPRESSO (QE) virtual hackathon: QE Coding Fridays

Venue and date: online on January 15 (14:00-18:00), January 22 (14:00-18:00), and January 29 (14:00-18:00), 2021

Organisers: the QE developers team.

Speakers: Paolo Giannozzi (SISSA), Filippo Spiga and Louis Stuber (NVIDIA).

Topics: Update about the status of the Quantum ESPRESSO distribution; work on different topics to advance the development of the distribution; if possible, solve some of the open issues on Gitlab; decide the developments' plans for 2021.

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

N of participants: 39

Overall assessment: General talks for all the participants were given at the beginning of the first two days. The first on the summary of main QE developments during 2020, plans for

2021, while the second was a showcase on how to use Profiling QE-GPU tools using Nsight. Next, the developers were divided into groups working connected in Zoom breakouts rooms, each one working on different topics coordinated by an experienced developer. Specific topics were: Merge of CPU and GPU distributions & GPU in linear-response codes, enhancement and documentation of the Time dependent Density Functional Perturbation Theory module, redesign and enhancement of the DFT+U module, general improvements in stability and robustness of selected modules. The hackathon meeting was also an opportunity for the developers to work on improvements of specific features for their current scientific projects, and the outcome of such developments entered the developers' branch of the code. A detailed report can be found here.

Program:
https://lists.quantum-espresso.org/pipermail/developers/attachments/20210122/c5a3b99b/attachment-0001.pdf

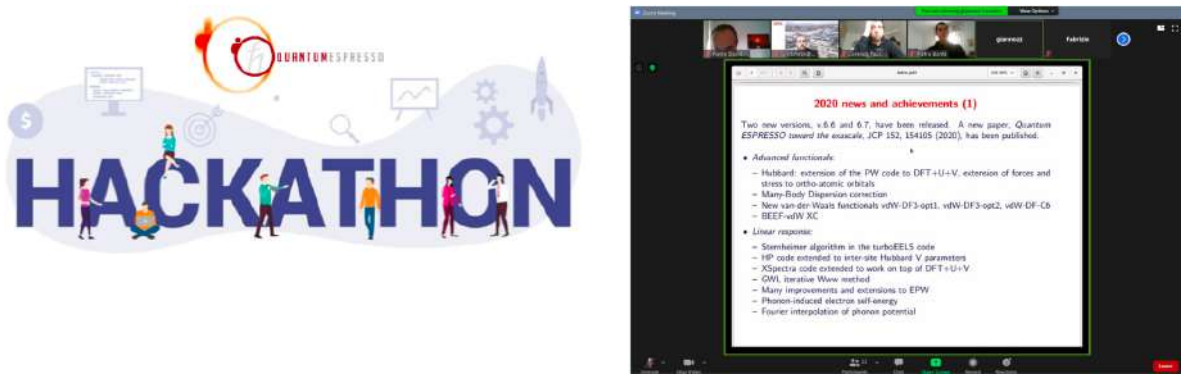

Fig 14. The promotional banner (on the left) and a moment (on the right) of the Quantum ESPRESSO virtual hackathon: QE Coding Fridays on new features and achievements

3. ESL Workshop 2021: Extended Software Development Workshop: Improving bundle libraries

Venue and date: CECAM-HQ-EPFL, Lausanne, Switzerland, October 11-22, 2021.

Organisers: Emilio Artacho (University of Cambridge), Volker Blum (Duke University), Micael Oliveira (MAX Planck Institute for the Structure and Dynamics of Matter), Nick Papior (Technical University of Denmark), Yann Pouillon (Simune Atomistics).

Speakers: Marc Torrent, Giovanni Pizzi, Susi Lehtola, Michele Ceriotti, Balint Aradi, Alan O'Cais, Alfredo Correa, Layla Martin-Samos, Alberto Garcia, Arash Mostofi, Stefano de Gironcoli, Yi Yao, Anton Kozhevnikov, Micael Oliveira, Irina Lebedeva, Paul Saxe, Alexander Buccheri.

Topics: the Electronic Structure Library (ESL) community organises 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 10 days of coding session) was devoted to setting up a common and consistent code development infrastructure / training in terms of compilation, installation, testing and documentation, that can be used seamlessly beyond the electronic structure community, and learn from solutions adopted by other communities. It also aimed at agreeing on metadata and metrics that are relevant for users of ESL components as well as third-party software, not necessarily related to electronic structure in a direct way. Creating long-lasting synergies between stakeholders of all communities involved and making it attractive for industry to contribute.

MAX Members: Stefano De Gironcoli (SISSA) discussed New developments of the Quantum ESPRESSO code: a combined CUF-OpenACC approach. Alberto Garcia (CSIC) discussed challenges and opportunities in Library Integration in Siesta. Giovanni Pizzi (EPFL) illustrated the Aiida platform, the Materials Cloud project and common workflows for materials properties. Anton Kozhevnikov (ETHZ) discussed the GPU accelerated plane-wave DFT library SIRIUS.

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

N of participants: 37

Website: https://www.cecam.org/workshop-details/23

4. AiiDA Coding Week

Venue and date: Hôtel Central Résidence, Leysin, Switzerland and online, December 6 - 10, 2021.

Organisers: AiiDA developers team.

Speakers: AiiDA developers team.

Topics: a few discussion or work topics had been identified before the start by the AiiDA team, and were addressed during the week. In particular, the following topics were discussed, and the result summarised in a set of draft documents for later implementation:

to overview and compare the different technologies we can use for task farming of jobs; to discuss the ways of moving the materials-science datatypes out of aiida-core; how push/pull for sharing AiiDA graphs with collaborators could work; the Web API for using AiiDA (AiiDA as a service); how to support an object-store backend for file repository; plans to remove the dependency on rabbitmq from aiida-core.

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

N of participants: 10 in person and few more online

Overall assessment: The week was characterised by lively discussion and active coding. Participants also had a great team-building opportunity, a lovely social dinner on Tuesday evening. The outcomes of the week and the feedback from the participants indicate also that similar events should be organised again, either online or on-site, the latter preferably if possible. A detailed report is available here.

Website: https://www.aiida.net/aiida-coding-week-2021/

Fig 15. Group picture of the AiiDA Coding Week 2021

5. Hackathon Porting MAX flagship codes on AMD accelerated architectures

Venue and date: fully online from January 27 to February 20, 2022

Organisers: Ivan Girotto (ICTP), Daniele Varsano (CNR), and Andrea Ferretti (CNR).

Speakers: George S. Markomanolis (CSC), Giacomo Rossi (INTEL), Stanimire Tomov (Innovative Computing Laboratory, University of Tennessee), Mark Gates (University of Tennessee), Piotr Luszczek (University of Tennessee).

Participants: Pietro Delugas (SISSA, QE), Oscar Baseggio (SISSA, QE), Nicola Spallanzani (CNR, Yambo), Daniel Wortmann (FZJ, Fleur), Andrea Ferretti (CNR, Yambo), Fabrizio Ferrari Ruffino

(CNR-IOM, Yambo), Andrea Marini (CNR, Yambo), Davide Sangalli (CNR, Yambo), Ivan Carnimeo (SISSA, QE), José M. Escartín (ICN2, SIESTA), Alberto Garcia (ICN2, SIESTA).

Topics: In this hackathon, selected members from the developers' group of the MAX flagship codes tested the accelerated versions of their application on AMD based platforms. Accelerated nodes equipped with AMD GPUs were made available by E4 (hosted at CINECA) and by CSC. The main objective was to preliminarily evaluate the performance and the effort required to run accelerated versions of MAX flagship codes on AMD accelerated architectures. In particular, as all accelerated versions of the MAX flagship codes are based on a combination of FORTRAN and OpenACC, the developers tested how the software stack installed on the available architectures supports these kinds of codes. The outcome of this hackathon provided an outlook of the expected behaviour - at least on a single node level - of the accelerated applications on the next coming EU pre-Exascale LUMI platform.

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

N of participants: 12

Overall assessment: the software technology available on AMD accelerated platforms tested at the time of the hackathon resulted in an early stage, especially considering compilers and wrappers related to FORTRAN codes. However, this had been for most participants the first approach to AMD accelerated platforms and software environment. Bases for collaborations were established during the hackathon, such that developers of the MAX flagship have followed up the effort of porting codes to AMD accelerated platforms on LUMI together with CSC staff along with AMD staff members.

Website:
http://www.max-centre.eu/news/max-hackathon-porting-max-flagship-codes-amd-accelerated-architectures

Fig 16. The promotional banner (on the left) and a slide on MAGMA today (on the right) of the Hackathon Porting MAX flagship codes on AMD accelerated architectures

6. Co-Design for HPC in Computational Materials and Molecular Science

Venue and date: CECAM-HQ-EPFL, Lausanne (CH), October 3 - 5, 2022

Organisers: Jose Maria Cela (BSC), Albert Farres (v), Andrea Ferretti (CNR), Claudia Filippi (University of Twente), Julio Gutierrez (v), Erwin Laure (MPCDF), Erik Lindahl (Stockholm University), Matthias Scheffler (Fritz-Haber-Institut der Max-Planck-Gesellschaft).

Speakers: Andreas Grüneis (TU Wien), Min Li (Huawei Research Europe), Branislav Jansik (IT4Innovations, VSB Technical University of Ostrava), Jean-Marc Denis (SIPEARL), Anthony Scemama (CNRS), Xavier Vigouroux (Atos), Markus Rampp (Max Planck Computing and Data Facility (MPCDF), Estela Suarez (Jülich Supercomputing Centre), Fabio Affinito (CINECA), Carlo Cavazzoni (Leonardo), Giacomo Rossi (Intel Corporation Italia S.p.A.), Alberto Garcia (ICMAB-CSIC), Filippo Mantovani (BSC), Erik Lindahl (Stockholm University), Joost Vandevondele (ETHZ), Filippo Spiga (NVIDIA), Marco Govoni (ANL).

Topics: (1) existing examples of HPC co-design in materials and molecular science, (2) co-design of general purpose and domain-specific libraries, kernels, and mini-apps, and (3) the perspective of hardware manufacturers, integrators, and data centre owners; the workshop focused in particular on, and attempt to draw conclusions about: (1) the relationship between algorithms and computer architectures in materials science, (2) the connection between parallel programming technologies and runtime systems, and (3) the interplay of the above layers for a wide spectrum of computer architectures, within the selected scientific domain.

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

N of participants: 22

Website: https://www.cecam.org/workshop-details/1113

Fig 17. Group picture of the Co-Design for HPC in Computational Materials and Molecular Science 2022

2.3 Visualisation and digital learning schools

- **Optimizing Digital Teaching and Communication**

Venue and date: online, from September 15 to October 1, 2021

Organisers and speakers: 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).

Topics: this hands-on workshop on e-learning techniques and strategies was held in September 2021, 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 organising 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 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 organisers 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.

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

N of participants: 16 (46 registered)

Overall assessment: After the last session, we presented an anonymous feedback form, where most of the questions were open ones: Many participants appreciated the variety of tools and techniques that were presented. Most participants were satisfied with the present content, but some indicated that more attention to sharing handwritten content could be a useful addition. Similarly, about creating graphical content, and more step-by-step guidance for creating a learning path. Most of the participants appreciated the organisation, the diversity of testimonies and applications, the vivid interaction among participants (during the online sessions and during the group homework). A detailed report can be found here.

Website: https://www.cecam.org/workshop-details/6

Fig 18. The promotional banner (on the left) and a group picture (on the right) of the Optimising Digital Teaching and Communication school 2021

2.4 Training Booklet

All the training material, including video lectures of the MAX training events, was collected and made available in the training section of the MAX webpage and MAX YouTube channel. In order to disseminate the training materials produced during 2021, essential pieces of information were collected in a virtual booklet permanently available online at

http://www.max-centre.eu/max-training-booklet and deposited in the Zenodo repository.

Fig 19. Pages from the Training Booklet.

The booklet contains all the useful information about the performed activities plus:

- Reports;
- Links to available training materials (such as abstracts, recorded lectures);
- A “facts and figures” final section.

The booklet was promoted on the project webpage and social media, Twitter and LinkedIn. It has been visualised 350 times and downloaded from Zenodo almost 140 times.

An overview of the booklet is also available in D9.4 (section 5.3 Graphically-designed materials).

Psi-k 2022. The booklet and the training activities have been presented to the community at the Psi-K 2022 conference, organised in Lausanne (Ch) on August 22-25, 2022. MAX organised several dissemination activities at the conference, such as a booth, in which the training materials (and Lhumos) were promoted, and a MaX event (the “MaX Happy Hour”) in which the main code developer from the project met their users in a friendly environment to answer code-specific questions or to present its multifaceted activities. Training had a dedicated table for meeting users.

Fig 20. MaX booth at Psi-K 2022 conference.

2.5 Participants statistics and considerations for future activities

As done in the first period, 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. The satisfaction of the attendees is measured every time through an anonymous feedback questionnaire.

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 different surveys for each school, reached a very positive evaluation of 4.6/5.

Altogether, the training events (schools, tutorials, hackathons) counted 1467 participants, and an overview of their responses is given below.

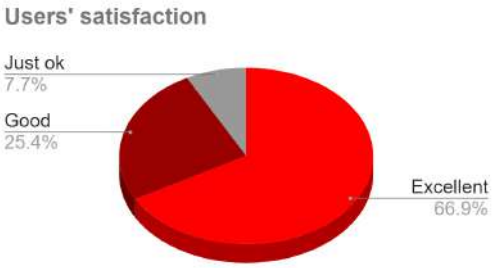

Fig 21. MAX training activities: user's satisfaction.

Overall, 5.4% of participants came from the countries of the EU13 area and 62.2% from outside Europe. The remaining 32.4% came from other European countries. Compared to the events held in the first 18 months, the presence of participants from outside Europe

significantly increased, due to the fact that most of the events were carried out remotely and this facilitated their participation. These data shows, however, that there is a strong interest in MaX codes on a global scale. To enlarge the pan-European participation in training initiatives, MAX included in its original training plan 3 events to deliver in Eastern Europe. Due to the pandemic, two of these events could not take place and were converted to online format, one of these events (Online tutorial on running and writing workflows with AiiDA, 2021, see above), experts from the Vilnius University were involved in the organisation of the event.

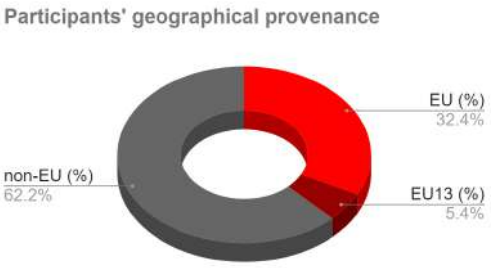

Fig 22. MAX training activities: participant's geographical provenance.

Within the pool of participants, 22.8% of the total were women, while the percentage of women that delivered the training (hands-on sessions tutors and lecturers) was 13.8%.

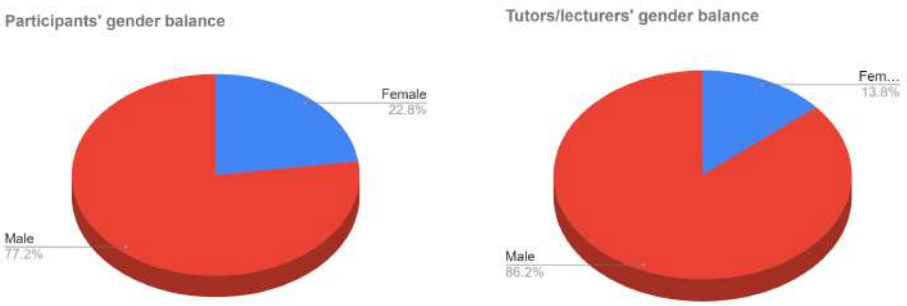

Fig 23. MAX training activities: participant's gender balance and tutors/lecturers' gender balance.

Different actions were put in place to address the gender imbalance, both in the phase of selection of the participants of the training events and in the list of lecturers and tutors. Despite the actions taken, the presence of a strong imbalance that needs to be mitigated is

evident, above all from the students' perspective. While it is possible to balance genders in the pools of lecturers (e.g., in the Yambo school (event n. 8) the gender representation was 40%), the observed imbalance in students' distribution most often reflects the gender imbalance of applicants, who were almost all accommodated in online events. Going back to in-person schools, and consequently to a limited number of students, a careful selection will be made respectful of gender balance and inclusivity at large.

Starting from the High Level Consulting services that MAX offers, industries often request "face-to-face" training for its employees, and this becomes a key part of subsequent contracts. In particular, ICN2 MaX partners continued its collaboration with the ISV SIMUNE. In the context of a service contract with ICN2, SIMUNE received training from ICN2 staff on the use of the SIESTA flagship code in systems with relevant spin-orbit interactions. Training sessions for some 80 person-days by ICN2 staff were delivered on this topic. Additionally, Prof. Pablo Ordejón (from ICN2) has been co-directing (together with Dr. Monica García-Mota, from SIMUNE) the research work of an employee of SIMUNE (Mrs. Jinxuan You), who is working towards her PhD on the topic of the study of proximity effects between magnetic materials and 2D topological insulators. This training effort has been sustained since 2020, and the PhD is expected during the first months of 2023.

MAX (CNR) continued to provide training and support to the Air Liquide company. The dedicated training concerned the use of the AiiDA framework together with the Quantum ESPRESSO suite of codes. The strategy followed by CNR-NANO to deliver the training about AiiDA and Quantum ESPRESSO was to organize tailor-made tutorials by exploiting scientific use cases of interest to Air Liquide. The first tutorial was related to the installation and setup of the AiiDA framework. The initial intention was to carry out this tutorial directly on the AL cluster and then to provide detailed documentation on the steps performed, highlighting the specific needs for the targeted cluster. However, due to the pandemic in progress, we decided to run the tutorial on a virtual machine hosted on Cineca servers.

The second tutorial was focused on how to use AiiDA to perform a relaxation run with the code PWscf configured in the previous tutorial. Subsequent meetings were dedicated to create a group of python scripts useful to perform all the steps of the needed workflow of calculations. The final result was the development of an AiiDA plugin containing the AiiDA work-chain that collects automatically all the steps of the workflow and keeps track of the provenance of all the input and output data.

2.6 MAX contribution to EU transversal training initiatives

During the period 01/06/2020-30/09/2022 MAX members participated in regular meetings organised by FocusCoE where online training best practice, collective CoE, training and the training section of the "HPC in Europe" portal were discussed.

All the MAX training events were uploaded to the HPC training portal calendar.

On March 26, 2021 MAX contributed to the FocusCoE training session at EuroHPC Summit Week EHPCSW where CoE training activities/initiatives were disseminated.

Most of the training events were organised in collaboration with community organisations such as CECAM (9 events), Psi-K (5 events) and ICTP (3 events), EuroCC National Competence Centre Sweden (ENCCS) among others.

2.6.1 Lhumos

MAX is one of the promoters of **Lhumos**: a web-based archive for the training and dissemination material (videos, notes, presentations) for simulations and modelling of materials, and beyond, via high-performing computing preparing for the exascale transition.

The Lhumos archive is currently under development and it is jointly developed with CECAM and MARVEL. The new portal is based on the Clowder system. Clowder is a research data management system designed to support any data format and multiple research domains. The original system has been integrated with several bespoke features to facilitate upload and management of training content.

The new archive is developed as a flexible user interface and presents a user-friendly environment for uploading and viewing data (video-lectures, training materials), implements metadata control protocols and effective management of tags for content.

Fig 24. Lhumos' leaflet cover (on theright) and the tweet (on the left) promoting Lhumos live demos @ Psi-K Conference 2022.

The web portal has been presented for the first time during the Psi-K conference 2022 in Lausanne by Roberto Bendinelli (EPFL), the developer of the platform. Further promotion of the portal will be done after its official release in Q2 2023.

2.7 Participation of MAX members as lecturers in other schools

MAX training activity goes beyond in-house events and includes contributions to third-party schools and training events. In these events, the training expertise focused on MAX flagship code, including hands-on and best practice in the code usage in pre-exascale machines. The lectures offered by MAX members are listed below:

1. MARVEL distinguished lecture @EPFL online on November 7, 2020

   MAX members: Stefano Baroni (SISS)

   Subject: Gauge invariance of heat and charge transport coefficients

   https://memento.epfl.ch/event/marvel-distinguished-lecture-stefano-baroni/

2. Simulation Workflows in Materials Modeling – SWiMM 2021 workshop – online - 15-26/03/2021

   MAX members: Nicola Marzari & Giovanni Pizzi (EPFL)

   Subject: The AiiDA & Materials Cloud informatics platform for complex workflows

   https://www.cecam.org/workshop-details/27

2. Virtual 2021 School on Electron-Phonon Physics from first principles - Austin, USA 14-18/06/2021

   MAX member: Paolo Giannozzi (Cnr Iom)

   Subject: Density-Functional Perturbation Theory and Additional contributions to the code: Debug and code alignment with QE

   https://docs.epw-code.org/doc/School2021.html

3. Cecam workshop: Excitonic and competing orders in low-dimensional materials - online - 22/06/2021

   MAX member: Daniele Varsano (Cnr Nano) - invited talk

   Subject: Evidence of ideal excitonic insulator in MoS2 under pressure

   https://www.cecam.org/workshop-details/21

4. Workshop on “Water: Grand Challenges for Molecular Science and Engineering”, Telluride Science Research Centre, Telluride (US) - 13/07/2021

MAX member: Pablo Ordejon (ICN2) - invited talk

Subject: Addressing electrified metal-electrolyte interfaces with Non-Equilibrium Green's Functions

https://www.telluridescience.org/meetings/workshop-details?wid=953

5. CECAM-Workshop Virtual Materials Design 2021 - Session Materials acceleration – online - 20-21/07/2021

   MAX member: Nicola Marzari (EPFL) - invited talk

   Subject: Digital infrastructures for materials discovery: the convergence of databases, simulations, and accelerators

   https://www.cecam.org/workshop-details/1093

6. MSSC21 - London (UK), virtual edition, 20-24/09/2021

   MAX member: Andrea Ferretti (CNR) - Invited lecture on 24/09/2021

   MAX Codes: Yambo and Quantum ESPRESSO

   Subject: Coherent electron transport through molecular nanojunctions

   https://www.imperial.ac.uk/mssc/mssc2021/

7. Cecam workshop: Recent developments in quantum Monte Carlo - Rome, Enrico Fermi Research Centre - 22/10/2021

   MAX member: Daniele Varsano (Cnr Nano) - invited talk

   Subject: Evidence of ideal excitonic insulator in MoS2 under pressure

   https://www.cecam.org/workshop-details/1050

8. Extended Software Development Workshop: Improving bundle libraries, Lausanne, Switzerland - 11-22/10/2021

   1. *MAX member:* Giovanni Pizzi (EPFL) - contributed talk

      Subject: AiiDA, Materials Cloud, and common workflows for materials properties with 11+ different engines

   2. *MAX member:* Anton Kozhevnikov (ETHZ/CSCS) - contributed talk

      Subject: SIRIUS: a GPU accelerated plane-wave DFT library

      https://www.cecam.org/workshop-details/23

9. MolSSI Workshop on HPC in Computational Chemistry and Materials Science - Berkeley, CA, USA - 13/12/2021

   MAX member: Anton Kozhevnikov (ETHZ/CSCS) - contributed talk

Subject: Libraries for electronic structure community

https://wordpress.cels.anl.gov/molssi-hpc/

10. Colloquium @ Colloquium Series in Theoretical and Computational Physics (CSTCP) - Physics Department of the University of Trieste, Italy - 24/02/2022

    MAX member: Daniele Varsano (Cnr Nano) - invited talk

    Subject: Hunting excitonic instabilities in low dimensional systems

    https://www.youtube.com/watch?v=Kd9yHfA7WPc

11. Electrified solid/water interfaces - theory meets experiments workshop - Tegernsee (Germany) - 15-18/05/2022

    MAX member: Ernane de Freitas Martins (RMIT-ICN2) - Contributed talk

    Subject: A multiscale QM/MM + NEGF approach to address electrified metallic-water interfaces

    https://www.mpie.de/eswi22

12. Virtual 2022 School on Electron-Phonon Physics from first principles - Austin, USA 13-19/06/2022

    MAX member: Paolo Giannozzi (Cnr)

    Subject: Density-Functional Perturbation Theory and Additional contributions to the code: Debug and code alignment with QE

    https://epw2022.oden.utexas.edu/https://epw2022.oden.utexas.edu/

13. Present and future of hybrid quantum chemical and molecular mechanical simulations workshop - Lecco (Italy) - 20-23/06/2022

    MAX member: Ernane de Freitas Martins (RMIT-ICN2) - Contributed talk

    Subject: Electrified metallic-water interfaces from a QM/MM + NEGF approach

    https://www.cecam.org/workshop-details/1152

14. Xenes-4 & Epioptics-16, International School of Solid State Physics - Erice, Italy - 03/07/2022

    MAX member: Deborah Prezzi (Cnr Nano) - invited talk

    Subject: Illuminating low-D Materials: Insights into Electronic and Optical Spectroscopies from First Principles Simulations

    https://www.ism.cnr.it/it/news/archivio-news/item/92-epioptics-16.html

15. CECAM Flagship Workshop Virtual Materials Design - Karlsruhe Institute of Technology, Germany - 18-21/07/2022

    MAX member: Daniel Wortmann (Jülich) - invited talk on 19/07/2022

    Subject: All-electron DFT heading to exascale: new possibilities for virtual materials design

    https://www.cecam.org/workshop-details/1143

16. FAIRmat workshop on data quality in DFT codes Co-organized by NOMAD - online - 14/09/2022

    -*MAX member:* Gregor Michalicek (Jülich)

    -*Subject:* Challenges in comparing LAPW calculations and estimating their precision

    -*MAX member:* Alberto García (CSIC)

    -*Subject:* Participation in roundtable discussion

    FAIRmat workshop on data quality in DFT codes

    https://www.fairdi.eu/events/fairmat-workshop-on-data-quality-in-dft-codes

17. MSSC22 - London (UK) - virtual edition 19-23/09/2022

    MAX member: Andrea Ferretti (CNR) - Invited lecture on 23/09/2022

    MAX Codes: Yambo and Quantum ESPRESSO

    Subject: Coherent electron transport through molecular nanojunctions

    https://www.imperial.ac.uk/mssc/mssc2022/

2.8 Teaching modules in University

Another part of the MAX training plan is devoted to courses and seminars provided to undergraduate Master students and PhD students, as well as to 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 realised by MAX partners.

1. **Online course on Computational Materials Physics - UGent**

Period: yearly basis from September until December.

MAX Member: Stefaan Cottenier (UGent).

The 12-week free and open online course on the use of DFT, illustrated with the Quantum ESPRESSO code (and available at https://compmatphys.epotentia.com/) is taught as a course module at Ghent University on a yearly basis from the end of September until December. At other times of the year, the material is available for self-paced study. Students outside Ghent

University can join the course as voluntary online students, either during the supervised edition in the fall term or during the rest of the year in the unsupervised self-paced mode.

A new supervised edition starts on September 26, 2022 with a much improved digital learning environment.

N. of participants: Fall 2020 edition: 65 + Fall 2021 edition: 55 (number of people attending the entire course and getting a certificate). There is a much larger number of people (more than 1000) who completed part of the course – often the part they were specifically interested in, and got something meaningful out of this course during the past 2 years.

Remarks from the organiser Stefaan Cottenier: "I have seen by now many examples of students who got credits from their home institution for taking this course online. At Psi-k 2022, I met many young researchers who told me they took this course in the past years. For some it even turned out to be the decisive moment to pursue a PhD in the electronic structure field."

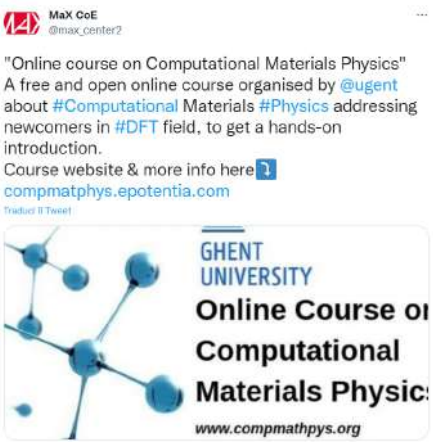

Fig 25. The MAX tweet promoting Online course on Computational Materials Physics - UGent.

2. **Hands-on course - Computational Laboratory of Quantum Mechanics** - University of Modena and Reggio Emilia, UNIMORE, Italy

Period: fall terms 2020/2021; 2021/2022

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

Number of participants: 15

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 of 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 specialised language. Furthermore, at the beginning of the course the students also acquired knowledge of basic Unix language and scripting and developed the ability to analyse 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.

A wiki page http://wiki.max-centre.eu/index.php/LabQSM was set up, edited, and updated by Andrea Ferretti and Daniele Varsano for the hands-on tutorial Laboratory of Quantum Simulation of Materials (LabQSM) within the Master degree in Physics of the University of Modena and Reggio Emilia (UniMoRe), fall terms (realised since 2016/2017).

3. **SISSA/ICTP Master in HPC (MHPC)**

Period: 8th edition 2021/2022 - 9th edition 2022/2023

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

Number of participants: 15 for each edition

MHPC is a 12-month program (from September to June + thesis project) structured in three parts. It is delivered by an international faculty composed by local HPC experts complemented by international well-renowned experts in the field.

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 PhDs and post-docs, and provides them with the technological background needed to master modern HPC applications. The first part of the program is dedicated to HPC technology, the second to the main computational problems on both HPC, AI and machine learning. A 6-month thesis on a practical project completes the course.

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).

4. **Contribution in the RWTH Aachen University Master Programme**

Period: winter semester 2020/2021, 2021/2022

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

Number of participants: 22, 11

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 part of the course 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.

5. **Course on Atomistic and Quantum Simulation of Materials** at EPFL

Period: spring semesters in 2020/2021; 2021/2022; 2022/2023

MAX members: Giovanni Pizzi (2022/2023), Nicola Marzari (EPFL), Francisco Ramirez as teaching assistant (EPFL).

Number of participants: 25 for each edition

University course at EPFL for Master/PhD students that covers basic topics of materials simulations: theory and application of quantum simulations to model, understand, and predict the properties of real materials. The course consists of 42 total hours of lectures and 14 total hours of computational labs practical work. This course featured the use of Quantum ESPRESSO and the QuantumMobile virtual machine.

https://edu.epfl.ch/coursebook/en/atomistic-and-quantum-simulations-of-materials-MSE-468

2.9 Training through research

Another successful channel of training is the “Training through research”. It means that academic and industrial researchers are hosted in the CoE labs. In these 28 months, overall,

20 young researchers were hosted in MAX Labs. This number is below the average of the first period due to Covid-19 restriction to travel and research exchanges.

The training visits organised in the CoE labs can be classified among different topics:

- a basic training on flagship code usage (Code Usage);
- an advanced training on flagship code related to a research project in computational materials science (Computational Materials Science);
- developing tools and libraries (Tools/libs development) for the flagship code, in order to implement new features in the codes for specific scientific needs.

In this training activity, MAX benefited from the synergy with the HPC-Europa3 program which funded 4 visits to MaX labs. The full list of researchers visiting MAX labs, host institutions, and purpose of the visit is given in Appendix 2.

2.10 Training on-demand

These training activities were organised to fulfill specific requests by institutions and other project networks.

- **BigMap on workflows and software 2020**

Period: December 2, 2020

MAX Members: Carl Simon Adorf, Marnik Bercx, Sebastiaan Huber, Giovanni Pizzi, Francisco Ramirez (EPFL)

No. of participants: 80

Basic usage of the Aiida platform and workflows for automated calculations for the H2020 BigMap consortium.

- **AiiDA tutorial @ Federal University of ABC, São Paulo, Brazil. 2021**

Period: February 2021

MAX Members: Flaviano Dos Santos (EPFL)

No. of participants: 20

Online Aiida tutorials for students of Federal University of ABC.

- **Python Course 2021**

Period: January 27-29, 2021

MAX Members: Nicola Spallanzani (CNR Nano)

No. of participants: 29

A short course on Python for HPC application for PhD students involved in the H2020 ERC TAME PLASMON project (University of Padova and University of Modena and Reggio Emilia).

- **AiiDA tutorial @ University of Antwerp, Belgium. 2022**

Period: May 2022

MAX Members: Marnik Bercx (EPFL)

No. of participants: 30

In-person tutorial at the University of Antwerp in Belgium on running AiiDA workflows using Quantum ESPRESSO.

3. Online training activities: webinars

MAX organised a webinar series presenting the latest developments of its flagship codes, their usage, and the perspective of use and performance of MAX codes on heterogeneous architectures, in view of the forthcoming EuroHPC machines. In the previous deliverable D8.2 we described the first two webinars dedicated respectively to Quantum ESPRESSO and AiiDA. Below you can find the description of the other 5 appointments:

1. Yambo webinar, 16/06/2020
2. CP2K webinar, 24/06/2020
3. SIESTA webinar, 22/09/2020
4. FLEUR webinar, 14/10/2020
5. BigDFT webinar, 12/11/2020

Yambo. The third webinar was dedicated to the quasiparticle band structures and excitons in novel materials using Yambo and took place on 16/06/2020.

Fig 26. The banner of the third webinar of the MaX series.

The main topics discussed during the webinar were the capabilities and features of the Yambo code tools for excited states calculations, with a particular focus on quasiparticle band structures and excitons in novel materials.

Speakers: Daniele Varsano (CNR), Andrea Marini (CNR), Maurizia Palummo (University of Rome Tor Vergata), Myrta Grüning (Queen's University Belfast), Andrea Ferretti (CNR).

Attendance: **185 active participants**. The average engagement degree was high.

Registered people: 245 people.

Interactions: **97 questions** were posed live to the speakers.

Poll Questions: during the webinar we set **4 Polls** (short & immediate surveys). These are the results coming out of 141 respondents:

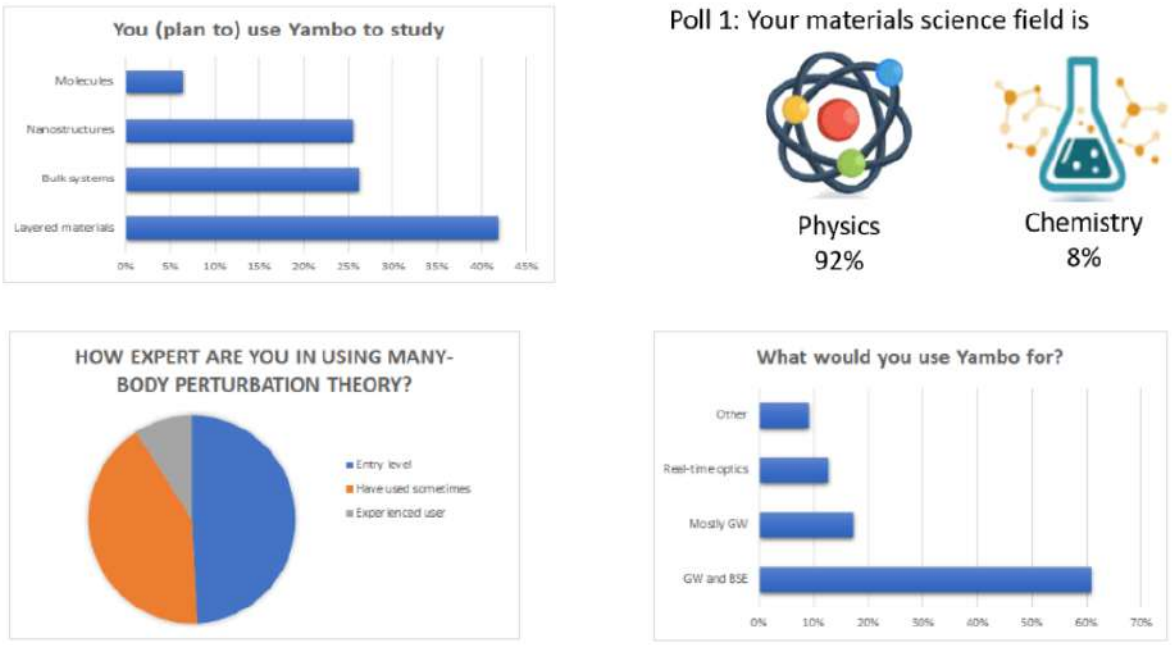

Fig 27. The results of the 4 poll questions of the Yambo code webinar.

Training materials: both the slides and webinar recorded video are now uploaded in the MAX dedicated Webpage for the benefit of the users and on MAX Youtube page as well.

CP2K. The fourth webinar was dedicated to HPC libraries for CP2K and other electronic structure codes and took place on 24/06/2020.

Fig 28. The banner of the 4th webinar of the MAX series.

The webinar provided an accurate overview of the HPC libraries developed at CSCS in order to accelerate electronic structure code such as CP2K and Quantum ESPRESSO. These libraries are (1) DBCSR, (2) COSMA, (3) SpFFT and (4) SIRIUS.

Speakers: Anton Kozhenikov (CSCS), Shoshana Jakobovits (CSCS), Marko Kabic (CSCS), Simon Frasch (CSCS).

Attendance: **80 active participants**. The average engagement degree was high.

Registered people: 126 people.

Interactions: **21 questions** were posed live to the speakers.

Poll Questions: during the webinar we set **3 Polls** (short & immediate surveys). These are the results coming out of 56 respondents:

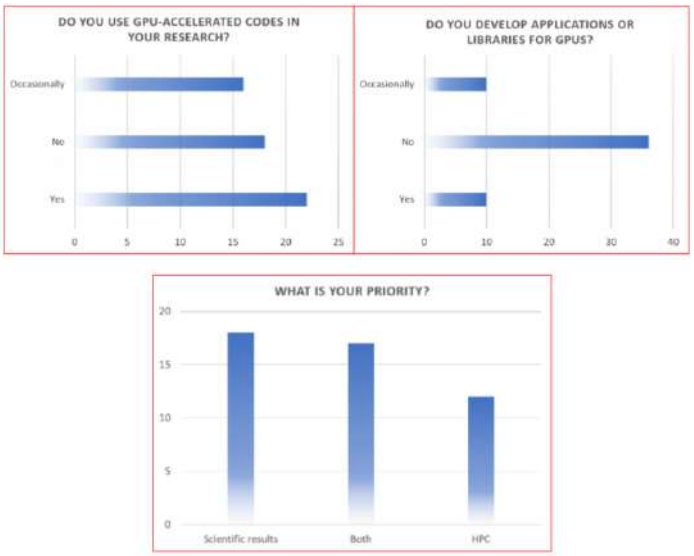

Fig 29. The results of the 3 poll questions of the CP2K code webinar.

Training materials: both the slides and the webinar recorded video are now uploaded in the MAX dedicated Webpage for the benefit of the users and in MAX Youtube page as well.

SIESTA. The fifth webinar was dedicated to the new developments in SIESTA for high-performance materials solutions and took place on 22/09/2020.

Fig 30. The banner of the fifth webinar of the MaX series.

The main topics discussed were the TranSIESTA built-in module, which implements a formalism based on non-equilibrium Green's functions, the latest improvements in its functionality (in particular multi-electrode support) and optimisation, user support within the SIESTA ecosystem.

Speakers: Emilio Artacho (Univ. of Cambridge and Nanogune), Alberto García (ICMAB-CSIC, Barcelona), Pablo Ordejón (ICN2, Barcelona), Nick Papior (DTU, Denmark), Mónica García-Mota (Simune Atomistics SL, San Sebastian).

Attendance: **151** online participants

Registered people: 213

Interactions: 55 live questions

Poll Questions: 5 poll questions

Training materials: both the slides and the webinar recorded video are now uploaded in the MAX dedicated Webpage for the benefit of the users and in the MAX Youtube page as well.

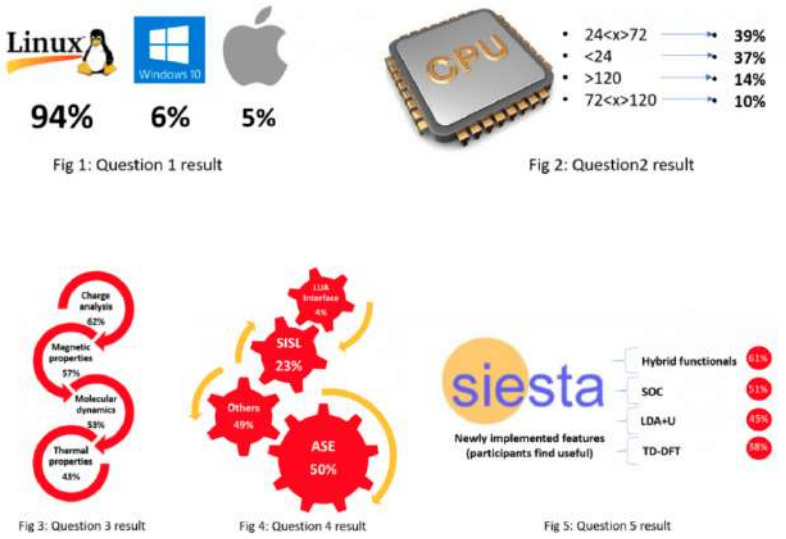

Fig 31. The results of the 5 poll questions of the SIESTA code webinar.

Fleur. The sixth webinar was dedicated to all-electron DFT using the FLEUR code and took place on 14/10/2020.

Fig 32. The banner of the sixth webinar of the MaX series.

The main topics were: basic features and fundamentals of the FLEUR code, the different types of simulations possible with the code, including its interfaces to other methods, the use of FLEUR on modern HPC systems including Tier-0 PRACE systems, hints and instructions useful for deploying FLEUR on different systems, and further sources of information, documentation and support processes and future plans of the code developers.

Speakers: Gregor Michalicek, Uliana Alekseeva, Daniel Wortmann (all Jülich).

Attendance: **100** participants

Registered people: 132

Poll Questions: 3

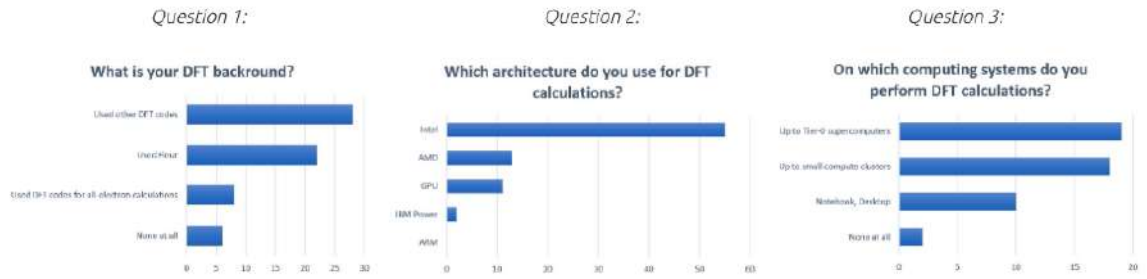

Fig 33. The results of the 3 poll questions of the FLEUR code webinar.

Training materials: both the slides and the webinar recorded video are now uploaded in the MAX dedicated Webpage for the benefit of the users and in the MAX Youtube page as well.

BigDFT. The seventh webinar was dedicated to the BigDFT code and the flexibilities wavelets for electronic structure calculations in large systems and took place on 12/11/2020.

Fig 34. The banner of the seventh webinar of the MaX series.

The main topics discussed were the features made possible by the peculiar properties of Daubechies wavelets, the usage of DFT for large-scale systems, the localised description of the KS problem and its role in providing a simplified description of large-scale electronic structure calculations.

Speakers: Luigi Genovese (CEA), Thierry Deutsch (CEA), Laura Ratcliff (Imperial College London), William Dawson (RIKEN), Augustin Degomme (CEA).

Attendance: **73** live participants

Registered people: 132

Poll Questions: 4

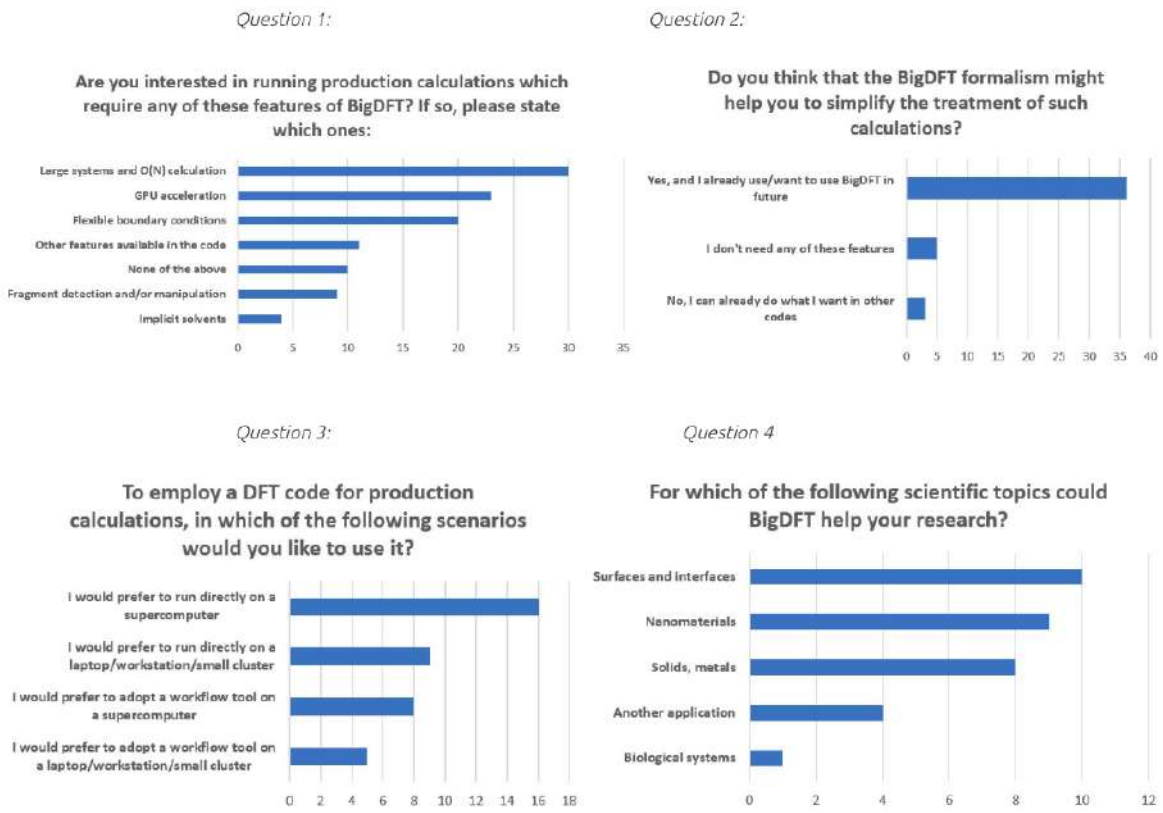

Fig 35. The results of the 4 poll questions of theBigDFT code webinar.

Training materials: both the slides and the webinar recorded video are now uploaded in the MAX dedicated Webpage for the benefit of the users and in the MAX Youtube page as well.

All the activities related to the MAX webinar series were collected in a virtual booklet permanently available online at http://www.max-centre.eu/max-webinars-booklet and on Zenodo. To date, the booklet has been visualized almost 450 times and downloaded 140 times from Zenodo.

An overview of the booklet is also available in D9.4 (section 5.3 Graphically-designed materials).

Fig 36. The cover of the Max code webinars' booklet.

4. 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 and to form a new generation of software developers in electronic structure and materials science.

In the M19-M46 period, we have continued to implement the actions described in the Training and Education plan that was previously outlined in D8.1 with few deviations from the original plan, mostly due to the COVID-19 pandemic. In particular, a large number of training events were reshaped and carried out in online formats.

All the training events organised for the MAX flagship code users and code developers (11 schools + 5 hackathons) were characterised by high participation of academic users and very positive feedback on the organisation, the provided training materials and the technology solutions employed for the online formats. These events were realised taking into account various priorities outlined in the training plan: the need of expanding the pan-European participation of users and institutions, the use of the virtual machine Quantum Mobile, containers and cloud platforms as it was highly encouraged many times (both in MAX schools and other events); the synergy in organising events with other EU infrastructures, such as CECAM, Psi-k, PRACE, National Competence Centres, 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 is still limited, confirming the trends already observed in previous years. When industrial users are interested in training in computational materials science and electronic structure they tend to opt for shorter and more focused training sessions, typically customised to the industry needs, dedicated, with tuition fees not being a key aspect. This aspect was confirmed by the training delivered by MAX towards the Air Liquide company and

ISV Simune which took place in this modality. The uptake by industrial users was however unsatisfactory, perhaps reflecting the still poor awareness of the potential of simulations in the HPC environment, but perhaps also the need to change communication strategies. Where the diffusion took place in a pushed way towards the industry (see webinars) the response of the industry was certainly greater as 17% of the participants were from industry, either ISVs or HW manufacturers.

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.

Despite the difficulties related to travel between different countries and within the same country in the latter period, MAX labs hosted 20 visiting students interested in working and learning the usage of the flagship codes, pointing out the high interest of the community in MAX partners' centres and codes.

Finally, MAX partners acquired a large experience in delivering online remote training which has been demonstrated allowing to broaden the audience and accept more students to single events. The training material, prepared on purpose for remote training, has been collected and made available in 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. We expect the collected material to be further used and disseminated once the Lhumos platform is up and running.

Appendix I

Feedback forms

After all the events organised by MAX, an anonymous standard feedback form was sent to the participants to quantitatively and qualitatively assess the course and, above all, to help the organizers understand what to improve the offer. For the online events, we also added questions regarding the satisfaction about the used technology.

In this section, for example, we report the results of the feedback received for two events, showing some statistics and some answers and comments by the participants.

Virtual school on electronic excitations in solids and nanostructures using the Yambo code (event 2, page 10)

Fig 37. Results of the "Course content rating" poll for Event 2 (page 10).

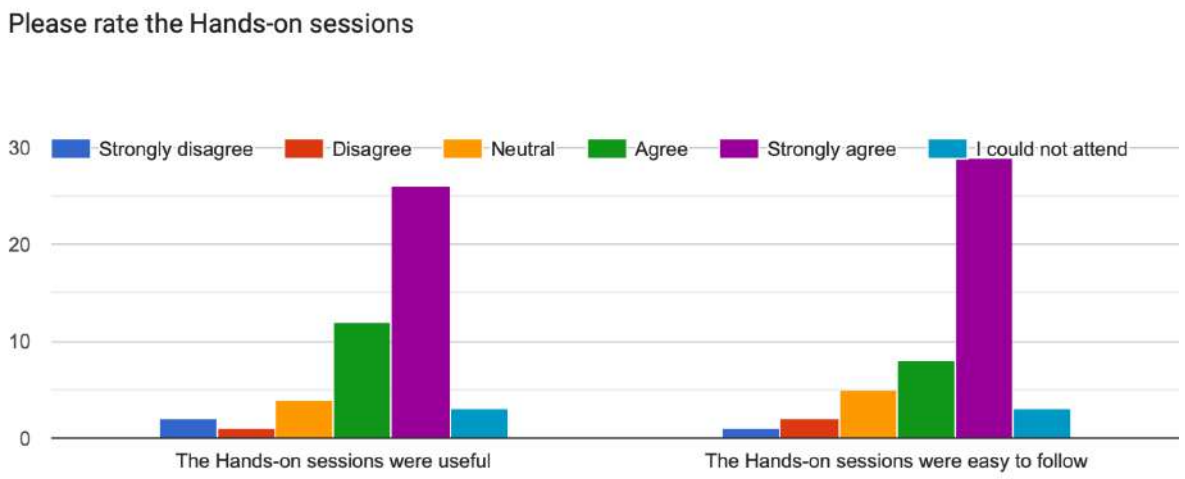

Fig 38. Results of the "Hands-on rating" poll for Event 2 (page 10).

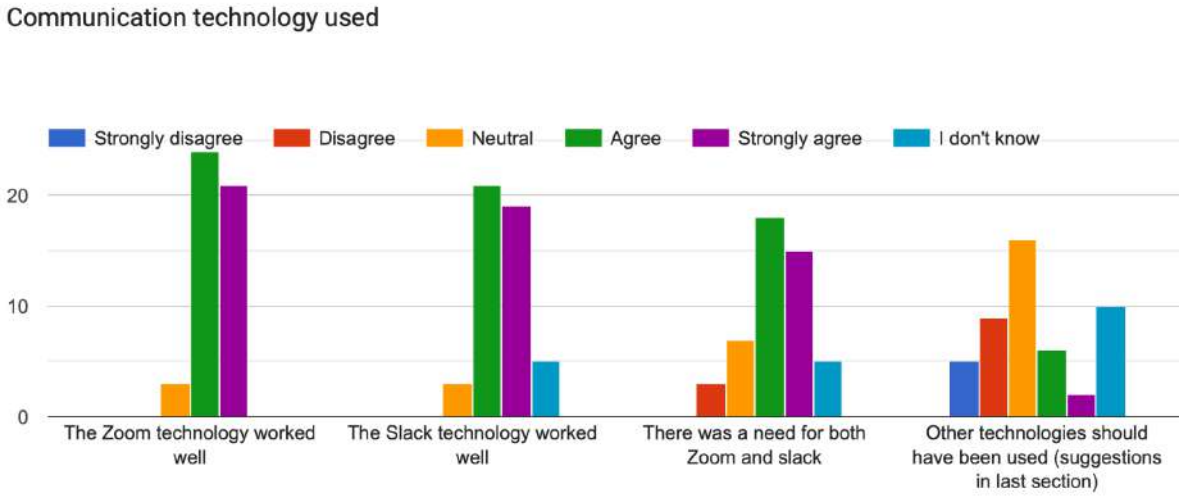

Fig 39. Results of the "Communication technology strategy rating" poll for Event 2 (page 10).

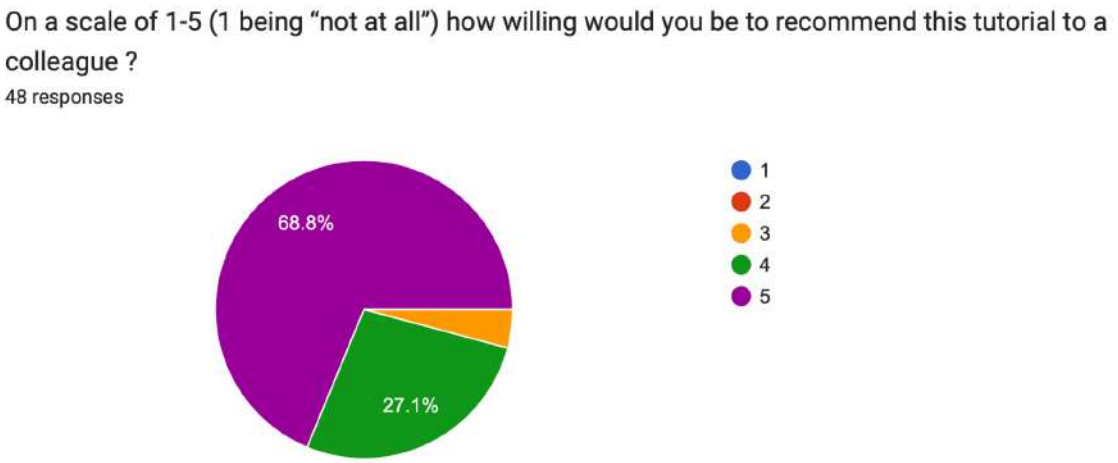

Fig 40. Results of the "Recommendation rating" poll for Event 2 (page 10).

Extracts of comments by attendants:

What aspects of this course were most useful or valuable?

- Reliability of advisors and sharing new knowledge
- Hands-on in small groups with knowledgeable tutors.
- Frequent questions and answer sessions, hands-on sessions.
- I had an idea about the calculation of excitonic properties from this school and It will be a good starting point to use Yambo in my research. Thank you very much to the organizers.
- Tutorials of very high quality followed by very useful practical sessions

How would you improve this course?

- A bit of YAMBO in practice mixed with the theory lectures. More interactive exercises.
- By awarding the students participating in course. We can arrange an assignment and can award students performing best in their assignment. This will encourage all participants.
- It is perfect already!

Any further comments (quality of the school, overall organization, suggestions on format, length, topics, on the YAMBO code itself, ...)

- The break-out rooms were really a plus to interact with instructors
- The school was well organized and well executed.
- Satisfactory but physical meeting would have been better
- Everything was good, but compared to lecture session I was engaged in tutorials
- It was wonderful, thank you! My only regret is that I won't get a Yambo t-shirt!

Online tutorial on running and writing workflows with AiiDA (event 7 page 17)

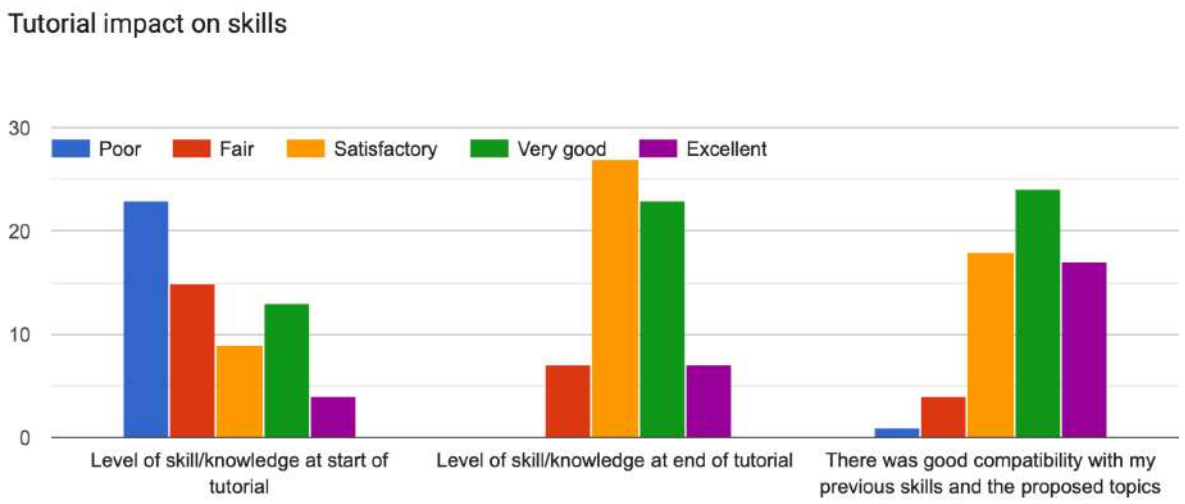

Fig 41. Results of the "Tutorial impact on skill rating" poll for Event 7 (page 17).

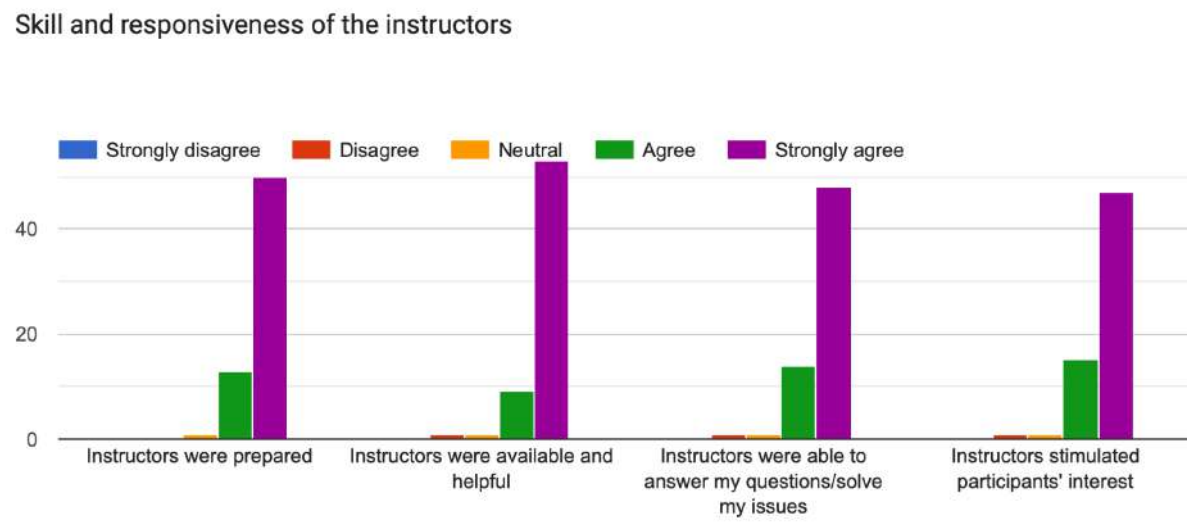

Fig 42. Results of the "Skill and responsiveness of the instructors" poll for Event 7 (page 17).

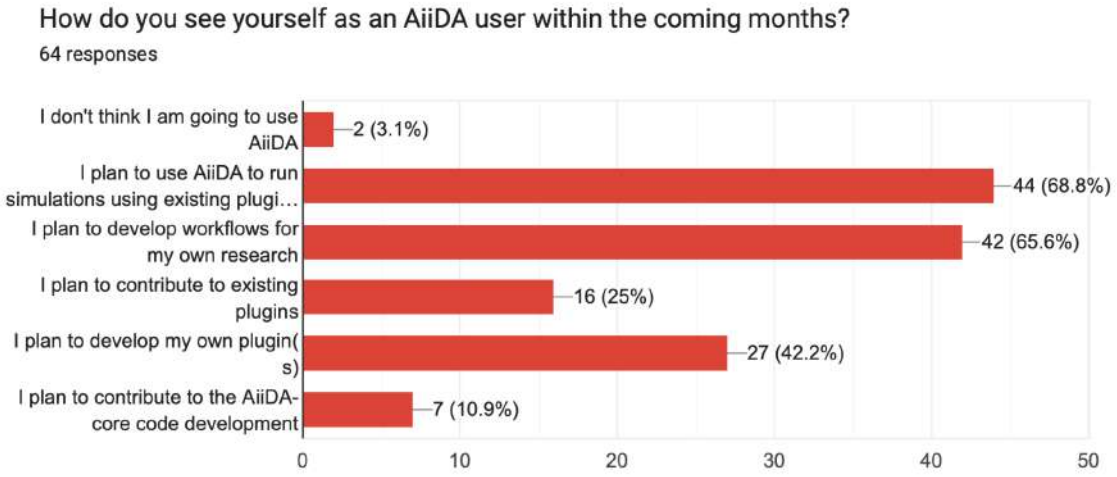

Fig 43. Results of the "Skill and responsiveness of the instructors" poll for Event 7 (page 17).

Extracts of comments by attendants:

What aspects of this course were most useful or valuable?

- Guideness and help from instructors on slack
- The course materials are well designed. The Jupiter hub setup is super helpful for starting up the tutorial.

- I think repetitions of concepts during the hands-on session was very useful to clear ideas
- Both the subject and the technologies used were interesting and edge-of-science and technology. I learned a lot!

How would you improve this course?

- I would make the course last longer (over more days) and evenly distribute task complexity so that the complete exercise can be more achievable in the set timeframe.
- A slightly longer duration (perhaps a week) is expected, for better comprehension of all the materials in the aiida-tutorial
- I would add more problem solving notebooks with different difficulties, which could be chosen by the participant.
- Perhaps in person would allow for more focus for a hackathon.

Any further comments (quality of the workshop, overall organization, suggestions on format, length, topics, on the AiiDA code itself, ...)

- Really enjoyed the workshop, high quality, skilled and helpful tutors, pitched at a good level.
- I just would like to thank all of you for your patience and willingness in teaching us and participating with us. I found it was the most engaging workshop I ever participated in.
- I think that the gather.town sessions were really great and fun! Not just for directly interacting with the AiiDA developers but also for meeting new people, sharing experiences and maybe collaborating in a specific way. Maybe regular sessions of this kind can be a fun way to hone a supportive AiiDA community across the globe, and I'd really enjoy making part of it :)
- Just one simple comment: Great! Thank you very much for making this course open to public.

Appendix II

List of researchers trained in CoE labs:

Guest: Federico Iori

Affiliation: Air Liquide SA

Hosting unit: CNR Nano (IT)

Period: 19/10/2020 - 27/11/2020

Purpose of the visit: Scientific research and technical support concerning the use of the MAX Centre of Excellence codes and training on electronic structure methods and related software.

Guest: Marc Gutiérrez Pérez

Affiliation: Universidad Autónoma de Barcelona

Hosting unit: BSC (ES)

Period: 01/03/2021 - 14/05/2021

Purpose of the visit: molecular dynamics research

Guest: Vijay Sudarshan

Affiliation: Technical University of Denmark

Hosting unit: EPFL (CH)

Period: 01/05/2021 - 01/09/2021

Purpose of the visit: Integration of AiiDA-QE plugin with ENVIRON

Guest: Lorenzo Bastonero

Affiliation: University of Bremen, Germany

Hosting unit: EPFL (CH)

Period: 15/09/2021 - 15/10/2021

Purpose of the visit: The AiiDA-hp plugin

Guest: Eric Macke

Affiliation: University of Bremen, Germany

Hosting unit: EPFL (CH)

Period: 15/09/2021 - 15/10/2021

Purpose of the visit: The AiiDA-hp plugin

Guest: Giovanni Cistaro

Affiliation: University of Madrid

Hosting unit: EPFL (CH)

Period: 15/09/2021 - 15/12/2021

Purpose of the visit: AiiDA

Guest: Lorenzo Varassi

Affiliation: University of Bologna

Hosting unit: EPFL (CH)

Period: 15/09/2021 - 15/12/2021

Guest: Carlo Cavazzoni

Affiliation: Leonardo spa

Hosting unit: CNR Nano (IT)

Period: 29/12/2021

Guest: Olamide Agbaoye Ridwan

Affiliation: Federal University of Agriculture, Physics Dep., Abeokuta, Nigeria

Hosting unit: CNR Nano (IT)

Period: 02/11/2021 - 27/01/2022

Purpose of the visit: *HPC-Europa 3* Training with the Yambo code for application in perovskite systems.

Guest: Gabriel Nascimento

Affiliation: Federal University of ABC, Brazil

Hosting unit: EPFL (CH)

Period: 01/02/2022 - 30/05/2022

Purpose of the visit: Protocols for 2D materials

Guest: Matteo D'Alessio

Affiliation: University of Mississippi, USA

Hosting unit: EPFL (CH)

Period: 01/02/2022 - 01/04/2022

Purpose of the visit: training on Aiida

Guest: Miki Bonacci

Affiliation: CNR Nano (IT)

Hosting unit: EPFL (CH)

Period: 15/02/2022 - 15/05/2022

Purpose of the visit: Development of the AiiDA-Yambo plugin

Guest: Pierre Lechifflart

Affiliation: Université de Marseille

Hosting unit: CNR Nano (IT)

Period: 28/02/2022 - 29/04/2022

Purpose of the visit: HPC-Europa 3 Implementation and optimisation of exciton-phonon coupling and photoluminescence in the Yambo code

Guest: Jacopo Rizzo

Affiliation: University of Roma, La Sapienza, Italy

Hosting unit: EPFL (CH)

Period: 01/04/2022 - 01/12/2022

Purpose of the visit: Quantum Computing

Guest: Changpeng Lin

Affiliation: EPFL

Hosting unit: CNR Nano (IT)

Period: 01/05/2022 - 08/06/2022

Purpose of the visit: developments of Yambo code

Guest: Marilia Caldas

Affiliation: University San Paolo

Hosting unit: CNR Nano (IT)

Period: 27/01/2022 - 05/03/2022

Purpose of the visit: HPC-Europa 3 Usage of Yambo code for defected systems

Guest: Samaneh Ataei

Affiliation: Department of Physics, Shahid Beheshti University, Tehran, Iran

Hosting unit: CNR Nano (IT)

Period: 06/06/2022 - 08/06/2022

Purpose of the visit: HPC-Europa 3 developments of Yambo code

Guest: Vittoria Urso

Affiliation: SISSA

Hosting unit: CNR Nano (IT)

Period: 20-21/06/2022 and 18/07/2022 - 22/07/2022

Purpose of the visit: developments of Yambo code

Guest: Wang Hao

Affiliation: Shandong University, China

Hosting unit: Juelich (DE)

Period: 15/12/2021 - 14/06/2022

Purpose of the visit: Calculation of topological and magnetic properties of 2D materials

Guest: Zhang Lishu

Affiliation: Humboldt Research Fellowship

Hosting unit: Juelich (DE)

Period: 01/08/2022 - 31/07/2024

Purpose of the visit: Investigation of transport in 2D spintronics materials

Guest: Freimuth Frank

Affiliation: Johannes Gutenberg Universität Mainz, Germany

Hosting unit: Juelich (DE)

Period: 01/01/2022 - 31/12/2022

Purpose of the visit: Moment-functional based spectral DFT