MaX DRIVING THE EXASCALE TRANSITION

MaX - Centre of Excellence

Training Booklet

2023-2025

MaX Training initiatives are a collective effort of all MaX members.

Training events coordination and data collection: Daniele Varsano, with the support of the MaX members involved in the training organization.

Editorial editing and content supervision: Marina Corradini, Luisa Neri, and Daniele Varsano.

Technical and graphical realization: Marina Corradini, Susanna Cavicchioli.

Table of Contents

Advancing expertise in HPC and computational materials science

Welcome to this collection of training activities organised by MaX – a community committed to empowering current and future experts in high-performance computing and computational materials science. As the field moves toward the exascale era, mastering advanced simulation tools has become key to tackling complex scientific challenges.

Through hands-on workshops, online learning resources, and collaborative research opportunities, MaX provides learners at all levels with the skills needed to use state-of-the-art materials modelling codes effectively. Alongside user training, we also invest in shaping the next generation of code developers, offering dedicated pathways for those who wish to contribute to the growth of the MaX open-source software ecosystem.

The booklet covers the schools, workshops, and learning opportunities organised by MaX between 2023 and 2025. It highlights our shared efforts to build a knowledgeable community ready to drive innovation in materials design and high-performance computing.

Daniele Varsano (CNR-Nano)
Coordinator of MaX Training and Education

Tackling emerging challenges in materials science research and computational modelling

In the world of computational materials science, progress depends on powerful tools and collaboration. MaX Centre of Excellence for Materials Design at the Exascale stands at the heart of this transformation. Its mission is to develop and refine a suite of advanced open-source codes that enable scientists to explore and predict the behavior of materials at the quantum level.

At the core of MaX work are five leading software packages: QUANTUM ESPRESSO, YAMBO, SIESTA, BigDFT, and FLEUR. Each of these codes plays a vital role in understanding different aspects of materials, from their electronic structure to their magnetic and optical properties. Together, they form a powerful ecosystem for quantum mechanical simulations.

Behind these tools is a dedicated **community of experts in high-performance computing and materials modelling**. They continuously test, optimise, and enhance each code, ensuring that every update delivers greater efficiency, reliability, and flexibility.

One of the defining features of the MaX codes is their **interoperability**. Scientists can combine them into complex workflows to enable large-scale simulations that go far beyond the capabilities of a single code. Whether studying the electronic structure of new materials, simulating advanced spectroscopic phenomena, or exploring magnetic properties, **scientists can rely on MaX tools to deliver accurate and scalable results**.

As computing technology advances toward the exascale era, MaX continues to play an important role in technological advancement. Its codes are regularly updated with new algorithms and scientific methods that make better use of next-generation supercomputers.

MaX work goes beyond developing software. It builds the technical framework that supports present and future research in materials science. With workflows designed for high-performance computing, MaX helps researchers study complex materials problems with greater accuracy and efficiency.

Training current and future professionals in HPC and materials science

At MaX, we believe that the future of materials science depends on people —researchers, students, and professionals — who can master the power of high-performance computing. Our mission is to help them build that expertise.

As computational materials science moves toward exascale computing, the ability to use advanced high-performance computing tools has become essential. We respond to this need by offering a **wide range of training opportunities, from hands-on workshops and hackathons to university lectures and tailored industry sessions**. Each activity is designed to give participants practical experience and the confidence to use MaX lighthouse codes effectively.

Our training program welcomes learners at every stage. We support those who are just starting to explore computational materials science, as well as experienced users looking to deepen their skills. Every session focuses on practical engagement, allowing participants to learn by doing and to understand how computational tools can solve real scientific challenges.

We also recognise the importance of flexibility in learning. For this, we offer **e-learning options** such as online courses, recorded lectures, and webinars. These resources make it easier for participants to learn at their own pace and stay connected to the latest developments in HPC and materials research.

To further support education, we organise dedicated schools and provide **open-access materials**, including lecture notes, tutorials, and guides related to MaX lighthouse codes. We also offer **internships** and **research training in MaX-affiliated laboratories** where participants can apply their knowledge in real-world projects.

Through these combined efforts, we aim to build a strong, skilled community ready to meet the challenges of modern materials science. By blending digital learning, hands-on practice, and collaboration, we help our users grow their expertise, strengthen their computational skills, and contribute to innovation in the field.

MaX knowledge hubs

MaX website

https://max-centre.eu/training/online-materials/

MaX website features a dedicated Training section that brings together a wide range of learning resources in HPC and computational materials science, designed for both early-career researchers and experienced professionals, including code developers and scientists from academia and industry.

Lhumos e-learning platform

https://www.lhumos.org/

Lhumos is an interactive training platform that offers a wide range of educational resources in HPC and computational materials science. Developed through a joint effort of European centres and organisations active in computational materials science, Lhumos provides video lectures, tutorials, and specialised training modules in a structured, user-friendly interface for learners at all levels of expertise.

MaX YouTube channel

www.youtube.com/@MaXCentreeXascale

MaX YouTube channel hosts recordings of MaX schools, training events, and past video lectures. Users can explore videos, playlists, lecture notes, and tutorials covering MaX flagship codes, HPC, and a wide range of materials science topics.

HPC in Europe portal

https://hpc-portal.eu/

The HPC in Europe portal provides a broad selection of learning materials and is regularly updated with new content to keep learners informed about the latest developments in the European HPC landscape.

Training Team

Lead: Daniele Varsano (CNR)

Core Members: Maria Bartolacelli (CNR), Susanna Cavicchioli (CNR), Luisa Neri (CNR)

Training Working Group

Chair: Daniele Varsano (CNR)

Node Representatives: Alice Ruini (UNIMORE), Oscar Baseggio (SISSA), José María Escartín Esteban (ICN2), Alberto García (CSIC), Gregor Michalicek (FZJ), Cristiano Malica (UBREMEN), Laura Bellentani (CINECA), Julio Gutiérrez (BSC), Karina Pešatová (IT4I), Anton Kokalj (IJS)

Hackathon Working Group

Coordinator: Oscar Baseggio (SISSA)

Committee Members: Daniele Varsano (CNR), Andrea Ferretti (CNR), Oscar Baseggio (SISSA; chair), Stefano De Gironcoli (SISSA), Daniel Wortmann (FZJ), Luigi Genovese (CEA), Alberto García (CSIC), Federico Pedron (ICN2), Fabio Affinito (CINECA), Lubomír Říha (IT4I), Ondřej Vysocký (IT4I).

Testimonials

Participating in the SIESTA school in 2024 was truly a great experience. The program included didactic lectures covering the most basic aspects of the code, as well as hands-on tutorials focused on data processing related to key topics in materials science, all guided by attentive and well-prepared tutors. It was a five-day event that greatly contributed to my academic development as a master's student in the field of nanomaterials.

Fernando Ribeiro Estigarribia Borges
Universidade Federal da Bahia, Brazil

I attended the YAMBO school as a PhD student whose research is mainly focused on simulations using Density Functional Theory. However, I am also interested in other ab initio techniques, and I was particularly curious about the YAMBO code. The school met my expectations: I enjoyed both the theoretical lessons and hands-on sessions, which I found very useful for understanding how the code works. I also enjoyed the social activities, which provided a great opportunity to connect with other PhD students and researchers. I hope to be able to use the YAMBO code in my future research!

Valentina Barreca
Università Federico II di Napoli, Italy

I was a participant in the SIESTA school in 2024 after using it for almost a year. I was really happy because all the lectures included both the basics for those who are starting from the very beginning and some more advanced tips that I did not know and that are extremely useful. Interaction was easy in every single tutorial thanks to the number of lecturers helping the students. Additionally, the event was completely free and can be attended online, so it was very easy to follow. I would recommend it for every SIESTA user, regardless of their level.

Jaime Garrido Aldea
ICN2, Spain

The YAMBO school was a great opportunity to understand the theoretical foundations that underlie the implementation of the code, while providing the practical notions for the correct use of the software in research work. The school enriched my knowledge on first principles methods based on

Green's function theory, and provided me with new concepts and practical instruments to improve my work as an early-career researcher.

Chiara Ribaldone
Università di Torino, Italy

I participated in the SIESTA summer school in 2024. The course was very well organised and beginner-friendly. Some sessions allowed participants to practise with the scripts provided, which I found very useful. Thanks to these courses, now I am getting more familiar with different functions of SIESTA. Looking ahead, I would be interested in some tutorials for post-analysis with an introduction to the common software needed.

Qiushi Deng
RMIT University, Australia

I attended the QUANTUM ESPRESSO School in Pavia in 2023, during the third year of my PhD. Having already some experience with the code and the underlying theory, I found the school extremely valuable for deepening my knowledge, and even more for clarifying subtle but important aspects of topics I was actively working on during my PhD. I could engage directly with the developers and leading experts in the field, and discuss my doubts in a very friendly and constructive environment. During the poster session, I could expand my network of collaborators, many of whom I'm still in contact with. Moreover, the hands-on sessions covered more advanced topics (such as Koopmans, DFT+U), allowing me to further expand my skills in QE.

Chiara Cignarella
EPFL, Switzerland

Attending the FLEUR Workshop 2023 as an early-career researcher was an excellent opportunity to deepen my understanding of FLEUR's theoretical foundations and advanced practical capabilities. The school fully met my expectations and significantly supported the progress of my research. Through direct interaction with the developers, I became familiar with sophisticated features of the code, and this contributed to publishing my ongoing projects in reputable journals. I highly recommend this workshop to anyone working with electronic-structure methods, especially in the field of magnetism.

Mohammad Amirabbasi
Technische Universität Darmstadt, Germany

As a young researcher, I joined the 2023 QUANTUM ESPRESSO (QE) School in Pavia to strengthen my skills in advanced DFT approaches. The focus on Hubbard and Koopmans functionals was highly relevant to my work on correlated and high-pressure materials, and the combination of theoretical lectures and hands-on training was very effective in highlighting the versatility and reliability of QE. It was also a unique chance to interact directly with QE developers, sparking ongoing discussions and collaborations that continue to shape my current research.

Francesca Menescardi
SISSA, Italy

I attended the YAMBO school in 2023, as an early career researcher, recognising it as a valuable opportunity towards advancing my research in complex Many Body Green function techniques. The school provided sound insights into the theoretical foundations as well as practical applications of the software, with nice and approachable lecturers and tutors. The school has surely met my expectations and also motivated me a lot to explore and learn more features of the software, thus allowing me to gain expertise in the same at a steady pace.

Manaswita Kar
Università di Modena e Reggio Emilia, Italy

I attended the YAMBO School in 2021 as an early-career researcher to include many-body perturbation theory in my research. The school provided comprehensive insights into the theoretical foundations and practical capabilities of YAMBO, fully meeting my expectations. It was also a fantastic opportunity to meet the developers, with whom I started collaborating to develop a self-consistent algorithm, which is essential to my research on topological materials. This new feature will be released soon.

Corentin Morice
Université Paris-Saclay, France
(former student, who later joined YAMBO as a developer)

MaX Training events

organised between 2023-2025

QUANTUM ESPRESSO

quantum-espresso.org/

QUANTUM ESPRESSO is an **open-source code** distributed under the GNU General Public License. It is a leading software suite used for **atomistic and electronic structure calculations**. Built on density-functional theory, plane waves, and pseudopotentials, it provides a flexible, modular, and high-performance platform for computational materials science.

The software includes a collection of core codes, plug-ins, and specialised applications. Researchers can perform energy and force calculations, study phonons through linear response, explore excitation spectra using time-dependent DFT (TDDFT), and carry out many other simulations.

QUANTUM ESPRESSO encourages global collaboration: scientists and developers from around the world can contribute, share improvements, and extend the software's capabilities. Through this collaborative approach, the platform continues to evolve, supporting cutting-edge research in materials modelling.

Date: 27-28/02/2023 **Venue:** Trieste (Italy)

QUANTUM ESPRESSO targeting accelerator

https://indico.ictp.it/event/10267/

The workshop combined training sessions with interactive discussions. It featured expert talks from major GPU card and compiler vendors, including Intel, AMD, and NVIDIA, alongside presentations from DevXlib developers. Developers shared their experiences, highlighting key advancements in porting FFTXlib and challenges encountered in distributed linear algebra integration. Each session concluded with open discussions, fostering collaboration and knowledge exchange among participants.

Participants: 18 (14M / 4F)

Partners: SISSA (IT), CNR (IT), CINECA (IT)

In collaboration with: ICTP (IT)

Organizer: O. Baseggio (SISSA)

Date: 28/08-01/09/2023 **Venue:** Pavia (Italy)

Advanced QUANTUM ESPRESSO school: Hubbard and Koopmans functionals from linear response

https://sites.google.com/view/hubbard-koopmans-2023/home?authuser=0

The school successfully introduced PhD students, postdocs, and junior scientists to cutting-edge approaches for modelling complex materials using first-principles methods. The program covered the fundamentals of DFT and density-functional perturbation theory (DFPT), focusing on extended Hubbard and Koopmans functionals. These approaches address key limitations in standard DFT, enabling more accurate ground-state and spectral property predictions. Participants engaged in theoretical lectures, technical presentations, and hands-on sessions using QUANTUM ESPRESSO, gaining practical skills in computing Hubbard parameters and Koopmans screening coefficients. The event fostered a deeper understanding of advanced DFT methods and equipped attendees with tools for their research and educational activities.

Applicants: 180 **Participants:** 41 (29M / 12F)

Training material:

Tutorials: https://github.com/materialscloud-org/QuantumESPRESSO-school-2023

Videolectures: https://lhumos.org/spaces/max

Partners: SISSA (IT), CNR (IT)

In collaboration with: Psi-K (UK), CECAM (CH), MARVEL (CH), Università di Pavia (IT)

Organizers: A. Ferretti (CNR), M. Cococcioni (Università di Pavia), N. Colonna (EPFL), and I. Timrov (PSI)

Date: 20-24/05/2024 **Venue:** Online

PWTK-2024: An Online Tutorial

http://pwtk.ijs.si/pwtk-2024.html

The PWTK-2024 online tutorial aimed to teach participants how to automate QUANTUM ESPRESSO calculations using the PWTK scripting environment. The program covered topics from basic scripting to advanced workflow creation, enabling users to employ built-in functionalities or develop custom scripts. The tutorial featured daily hands-on sessions, allowing participants to practice on their laptops or desktops with access to an HPC supercomputer.

Applicants: 152 **Participants:** 95 (71M / 24F) **Assessment:** 4.77/5.0

Training material:

Tutorials: https://repo.sling.si/tonek/PWTK-2024

Videolectures: http://pwtk.ijs.si/pwtk-2024.html

Partners: SISSA (IT), Jožef Stefan Institute (SI)

In collaboration with: EuroCC SLING (SI)

Organizer: A. Kokalj (IJS)

Date: 18-21/06/2024 **Venue:** Online

Materials and molecular modelling with QUANTUM ESPRESSO

https://events.it4i.cz/event/252/

The course provided a comprehensive curriculum covering the primary features of the QUANTUM ESPRESSO code, balancing theoretical concepts with practical applications. Designed for beginners and intermediate users, it offered hands-on training to develop essential skills for using the code in research and academic projects. Participants with backgrounds in condensed matter physics or chemistry learned key aspects such as code compilation, basic scripting, and parallelization strategies, enabling them to perform simulations effectively and interpret computational results.

Applicants: 201 **Participants:** 46 (32M / 14F) **Assessment:** 4.85/5.0

Training material:

Videolectures: https://www.youtube.com/watch?v=HknPlJzMmx0

Partners: SISSA

In collaboration with: NCC Austria, NCC Czechia, NCC Hungary, NCC Poland, NCC Slovakia, and NCC Slovenia

Organizers: O. Baseggio (SISSA) and K. Pešatová (IT4I, NCC Czechia)

Date: 12-13/11/2024 **Venue:** Zagreb (Croatia)

Modelling of (nano)materials with QUANTUM ESPRESSO

https://www.hpc-cc.hr/NCC_Croatia_HPC_day_2024

The workshop covered the key features of the QUANTUM ESPRESSO code, with an emphasis on developing practical skills in atomistic modeling using density functional theory methods. Participants gained hands-on experience applying these methods to real-world problems, focusing on practical applications. The goal was to equip attendees with the necessary skills to effectively use QUANTUM ESPRESSO on modern HPC systems in their research.

Applicants: 10 **Participants:** 8 (7M / 1F) **Assessment:** 4.83/5.0

Training material:

Tutorials: https://gitlab.com/kokalj/qe-workshop_ncc-croatia-2024

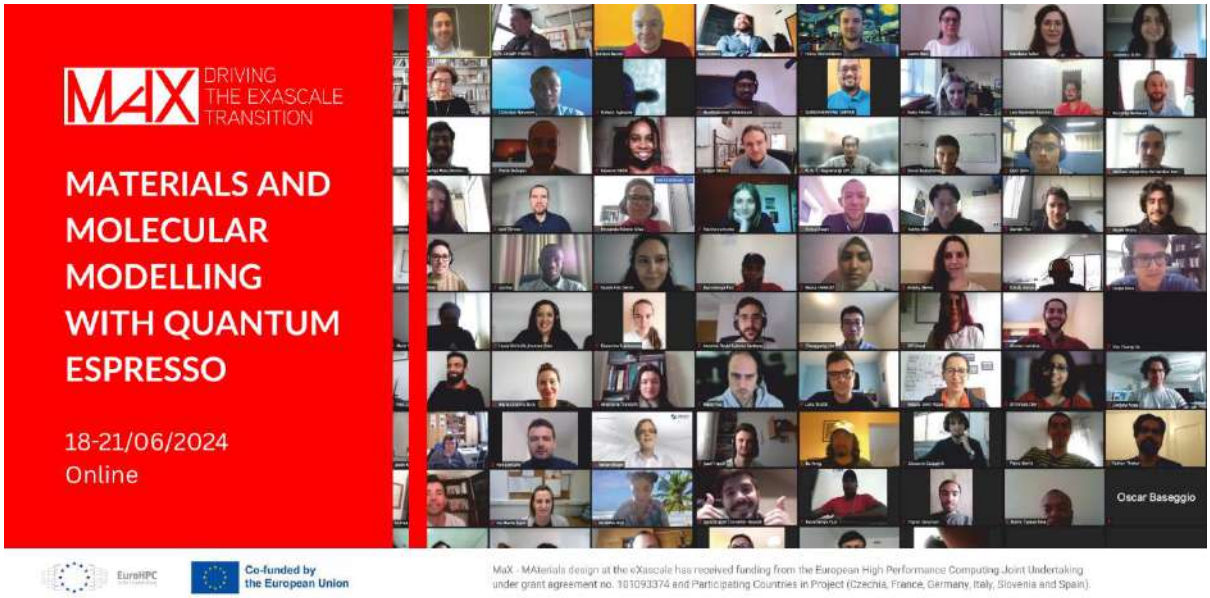
Partners: SISSA (IT), Jožef Stefan Institute (SI)

In collaboration with: NCC Croatia

Organizers: O. Baseggio (SISSA), A. Kokalj (IJS), M. Pobrežnik (IJS), and P. Delugas (SISSA)


DRIVING THE EXASCALE TRANSITION
QUANTUM ESPRESSO TARGETING ACCELERATOR
27-28/02/2023
Trieste (Italy)
EuroHPC
Co-funded by the European Union
MaX - MAterials design at the eXascale has received funding from the European High Performance Computing Joint Undertaking under grant agreement no. 101093374 and Participating Countries in Project (Czechia, France, Germany, Italy, Slovenia and Spain).


DRIVING THE EXASCALE TRANSITION
ADVANCED QUANTUM ESPRESSO SCHOOL
28/08 - 01/09 2023
Pavia (Italy)
EuroHPC
Co-funded by the European Union
MaX - MAterials design at the eXascale has received funding from the European High Performance Computing Joint Undertaking under grant agreement no. 101093374 and Participating Countries in Project (Czechia, France, Germany, Italy, Slovenia and Spain).


DRIVING THE EXASCALE TRANSITION
MATERIALS AND MOLECULAR MODELLING WITH QUANTUM ESPRESSO
18-21/06/2024
Online
Oscar Baseggio
EuroHPC
Co-funded by the European Union
MaX - MAterials design at the eXascale has received funding from the European High Performance Computing Joint Undertaking under grant agreement no. 101093374 and Participating Countries in Project (Czechia, France, Germany, Italy, Slovenia and Spain).

YAMBO

yambo-code.eu/

YAMBO is an **open-source software** released under the GPL license, designed to study the excited-state properties of materials from first principles. It is built on Green's function theory, offering advanced methods to understand complex material behaviour.

The code implements several key techniques, including the GW approximation, the Bethe-Salpeter equation (BSE), electron-phonon interactions, and non-equilibrium Green's function theory (NEGF). These tools enable researchers to calculate a wide range of physical properties with high accuracy.

With YAMBO, users can determine reliable band gaps, band alignments, defect quasiparticle energies, as well as optical and non-equilibrium properties. Its open-source nature encourages collaboration, allowing scientists worldwide to contribute and enhance its capabilities. This makes YAMBO a powerful platform for exploring the excited-state behaviour of realistic materials.

Date: 22-26/05/2023 **Venue:** Roma (Italy)

Ab-initio many-body perturbation theory: from equilibrium to time-resolved spectroscopies and nonlinear optics

https://www.yambo-code.eu/2023/02/18/yambo-school-2023/

The school focused on many-body perturbation theory approaches for first-principles simulations of excited states in materials using the YAMBO code. Advanced nonequilibrium techniques for ultrafast spectroscopy were also covered with the CHEERS code. Participants attended theoretical and technical lectures, complemented by hands-on sessions applying the codes to realistic simulations in the HPC environment. Core topics included quasiparticles through the GW approximation and excitons via the Bethe-Salpeter equation. Advanced discussions explored nonlinear optics and time-resolved dissipative dynamics using nonequilibrium Green's function theory. Each topic was introduced with relevant experimental contexts and clear connections to the practical exercises.

Applicants: 88 **Participants:** 39 (29M / 10F) **Assessment:** 4.64/5.0

Training material:

Tutorials: https://wiki.yambo-code.eu/wiki/index.php/Rome_2023

Videolectures: https://lhumos.org/spaces/max

Partners: CNR (IT), CINECA (IT)

Organizers: D. Varsano (CNR), F. Paleari (CNR), D. Sangalli (CNR), M. Grüning (Queen's University Belfast), M. Palummo (Università di Roma Tor Vergata), and A. Molina-Sánchez (Universidad de Valencia)

Date: 27-29/02/2024 **Venue:** Online

YAMBO-AiiDA plugin tutorial

https://www.yambo-code.eu/2024/01/12/yamboaiida/

The school provided in-depth training on automating many-body perturbation theory (MBPT) calculations beyond density functional theory (DFT). Participants explored efficient algorithms for GW and Bethe-Salpeter equation (BSE) simulations, including robust convergence procedures and a novel GW band interpolation method using maximally localised Wannier functions. Practical sessions focused on the AiiDA platform, enabling automation of GW convergences and band interpolation tasks. By the program's end, attendees had acquired the skills needed to advance materials discovery through state-of-the-art computational techniques.

Applicants: 66 **Participants:** 32 (23M / 9F) **Assessment:** 4.8/5.0

Training material:

Tutorials, slides of the presentations and a dedicated version of the quantum mobile are available at: https://www.yambo-code.eu/2024/01/12/yamboaiida/

Partners: CNR (IT), PSI (CH)

Organizers: D. Varsano (CNR), D. Prezzi (CNR), F. Paleari (CNR), M. Bonacci (PSI), M. Bercx (PSI), and A. Marrazzo (Università di Trieste)

Date: 26-28/11/2024 **Venue:** Modena (Italy)

YAMBO Hackathon

https://www.yambo-code.eu/2024/11/15/yambo-developers-meeting-2024/

The Hackathon was organised through a combination of presentations, discussions, and coding sessions. The presentations covered key updates on YAMBO capabilities, including improvements in linear algebra, electron-phonon coupling, and real-time simulations. Updates on the Yambo-py platform, along with new features and ongoing projects related to machine learning techniques, were also presented. The hackathon sessions focused on GPU porting, distributed GPU linear algebra, calculation of new observables (e.g., photoluminescence), and code maintenance. The event offered participants the opportunity to actively contribute to the YAMBO development and concluded with a session on preparing the next release of the code.

Participants: 34 (25M / 9F)

Partners: CNR-Nano (IT)

Organizers: D. Varsano (CNR), D. Sangalli (CNR), and A. Ferretti (CNR)

Consiglio Nazionale delle Ricerche

Date: 19-23/05/2025 **Venue:** Modena (Italy)

Many-Body Perturbation Theory and Excited-State Simulations

https://www.yambo-code.eu/2025/01/17/yambo-school-modena-2025/

The school focused on computational methods for studying light-matter interactions, essential for optoelectronics, quantum technologies, and energy research. Participants attended lectures on many-body perturbation theory, covering both basic and advanced topics. Key subjects included quasiparticles via the GW approximation, excitonic effects using the Bethe-Salpeter equation, and nonlinear optical simulations. Recent algorithms for 2D materials and metals were also discussed. Hands-on sessions provided experience with the YAMBO code in high-performance computing environments, including GPU-accelerated resources. Participants practiced Python-based post-processing and data analysis with the YamboPy toolkit. The program emphasized connecting theoretical concepts to experimental applications, ensuring a strong link between advanced theory and practical use in modern research fields.

Applicants: 70 **Participants:** 42 (30M / 12F) **Assessment:** 4.9/5.0

Training material:

Tutorials: https://wiki.yambo-code.eu/wiki/index.php?title=Modena_2025

Partners: CNR-Nano (IT), CINECA (IT)

In collaboration with: Psi-K (UK), CECAM (CH)

Organizers: D. Varsano (CNR), A. Ferretti (CNR), F. Paleari (CNR), D. Sangalli (CNR), A. Marini (CNR), E. Cannuccia (Aix-Marseille Université), C. Attaccalite (Aix-Marseille Université), and M. Palummo (Universitá di Roma Tor Vergata)

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AB-INITIO MANY-BODY PERTURBATION THEORY

22-26/05/2023
Roma (Italy)

EuroHPC Co-funded by the European Union

MaX - MAterials design at the eXascale has received funding from the European High Performance Computing Joint Undertaking under grant agreement no. 101093374 and Participating Countries in Project (Czechia, France, Germany, Italy, Slovenia and Spain).

MAX DRIVING THE EXASCALE TRANSITION

YAMBO DEVELOPERS' MEETING

26-28 November 2024

Modena (IT)

EuroHPC Co-funded by the European Union

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MAX DRIVING THE EXASCALE TRANSITION

MANY-BODY PERTURBATION THEORY AND EXCITED-STATE SIMULATIONS

19-23/05/2025
Modena (Italy)

EuroHPC Co-funded by the European Union

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SIESTA

siesta-project.org/siesta/

SIESTA is a DFT code designed from the outset to perform efficient simulations for large systems. SIESTA's efficiency stems from the use of a basis set of strictly-localised atomic orbitals, which leads to moderate matrix sizes in diagonalization and enables the use of low-complexity methods (e.g., linear scaling and the PEXSI scheme) that exploit sparsity.

A very important feature of the code is that its accuracy and cost can be tuned in a wide range, from very fast exploratory calculations to highly accurate simulations matching the quality of other approaches, such as plane-wave methods.

Date: 02-06/10/2023 **Venue:** Online

First steps with SIESTA: from zero to hero

https://www.cecam.org/workshop-details/first-steps-with-siesta-from-zero-to-hero-1240

The school provided hands-on training on the SIESTA code, in particular on essential theoretical foundations of DFT and practical sessions on using SIESTA effectively. Participants learned how to adjust the software's accuracy and computational cost. Training also included parallelization techniques, efficient solvers, and advanced features like quantum transport using the non-equilibrium Green's function (NEGF) approach. The event successfully equipped participants with the skills needed to perform advanced simulations and analyse results using pre- and post-processing tools.

Applicants: 156 **Participants:** 119 (84M / 35F) **Assessment:** 4.65/5.0

Training material:

Tutorials: https://siesta-project.org/siesta/events/SIESTA_School-2023/Sessions.html

Partners: ICN2 (ES), BSC (ES)

In collaboration with: CECAM (CH)

Organizers: S. Achilli (Università di Milano), E. Artacho (Nanogune, Ikerbasque and University of Cambridge), A. Cammarata (Czech Technical University in Prague), J.M. Escartín (ICN2), J. Gutiérrez (BSC), N. Papior (Technical University of Denmark), F.N. Pedron (ICN2), and M. Pruneda (CSIC)

Date: 11-15/11/2024 **Venue:** Online

SIESTA school 2024

https://siesta-project.org/siesta/events/SIESTA_School-2024/

The school offered practical training on the SIESTA software, attracting researchers and students from a wide range of scientific fields such as materials science, chemistry, and nanoscience. The program aimed to strengthen participants' capabilities in computational materials research. It provided a thorough introduction to the theoretical principles of density functional theory (DFT) alongside hands-on exercises to effectively utilize SIESTA. Attendees gained experience in balancing computational precision and performance, as well as learning parallelization strategies, efficient solver usage, and advanced functionalities, including quantum transport simulations via the non-equilibrium Green's function (NEGF) method. Overall, the school successfully empowered participants to conduct sophisticated simulations and interpret their results using both pre- and post-processing tools.

Applicants: 357 **Participants:** 151 (111M / 40F) **Assessment:** 4.66/5.0

Training material:

Tutorials: https://siesta-project.org/siesta/events/SIESTA_School-2024/Sessions.html

Partners: ICN2 (ES), BSC (ES), EuroCC Spain

Organizers: C. Coll (ICN2), J.M. Escartín (ICN2), R. Farris (ICN2), J. Gutiérrez (BSC), F.N. Pedron (ICN2), and M. Pruneda (CSIC and ICN2)

Date: 02-05/06/2025 **Venue:** Barcelona (Spain)

Advanced SIESTA workshop 2025

https://www.cecam.org/workshop-details/advanced-siesta-workshop-2025-1409

The workshop highlighted the capabilities of the software in exploring computational challenges often difficult for other density functional theory approaches. Over three days, experts presented state-of-the-art research and demonstrated SIESTA integration with complementary computational tools. Topics included advanced magnetic property calculations with TB2J, thermal conductivity via TDEP, electrochemical modelling using SIESTA QM/MM interface, potential energy surface explorations with SIESTA/LUA, and electron-phonon coupling studies through the elph interface. The workshop also showcased SIESTA performance in exascale and pre-exascale systems. The workshop offered a platform for researchers to advance their understanding of SIESTA applications and discuss innovative approaches in computational materials science.

Applicants: 77 **Participants:** 31 (24M / 7F)

Training material:

Tutorials: https://docs.siesta-project.org/projects/siesta/en/stable/

Partners: ICN2 (ES)

In collaboration with: Psi-k (UK), CECAM (CH)

Organizers: C. Coll (ICN2), J.M. Escartín (ICN2), R. Farris (ICN2), F.N. Pedron (ICN2), and M. Pruneda (CSIC)

❙ **Date:** 17-21/11/2025 ❙ **Venue:** Online

SIESTA school 2025

https://www.cecam.org/workshop-details/siesta-school-2025-1415

The school focused on electronic-structure calculations and ab initio molecular dynamics for molecules, nanostructures, and solids. It emphasised how to balance computational cost and accuracy for different types of simulations, from quick exploratory studies to highly precise calculations comparable to plane-wave methods. Through lectures and hands-on sessions, participants gained experience with the code's core functionalities, including parallelization strategies, modern solvers, and essential pre- and post-processing tools. The program introduced advanced topics, such as quantum transport calculations using the non-equilibrium Green's function approach, equipping attendees with the knowledge and skills to tackle both standard and cutting-edge research challenges using SIESTA.

❙ **Applicants:** 130 ❙ **Participants:** 97 (73M / 24F) ❙ **Assessment:** 4.57/5.0

Training material:

Tutorials: https://docs.siesta-project.org/projects/siesta/en/stable/

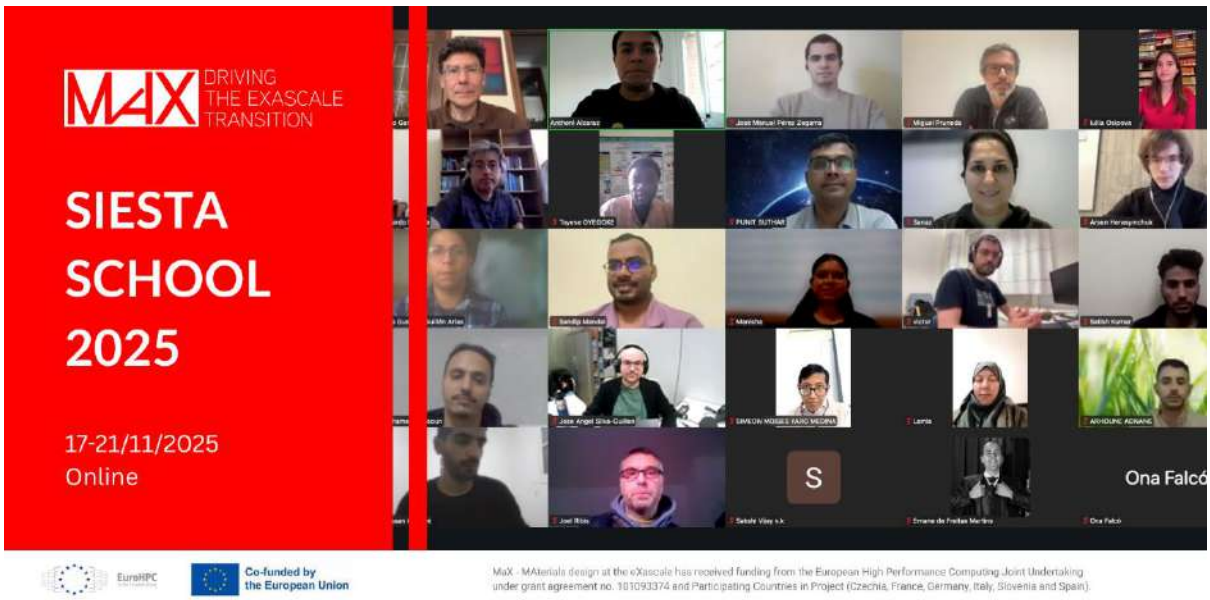
Partners: ICN2 (ES)

In collaboration with: CECAM (CH)

Organizers: J.M. Escartín (ICN2) and M. Pruneda (CSIC)


MAX DRIVING THE EXASCALE TRANSITION
SIESTA School 2024
11-15 NOVEMBER 2024
ONLINE
siesta
ICN2
Institut Català de Nanociència i Nanotecnologia
BSC Barcelona Supercomputing Center
CSIC
EuroHPC
Co-funded by the European Union


MAX DRIVING THE EXASCALE TRANSITION
ADVANCED SIESTA WORKSHOP 2025
02-05/06/2025
Barcelona (Spain)
EuroHPC
Co-funded by the European Union
MaX - MAterials design at the eXascale has received funding from the European High Performance Computing Joint Undertaking under grant agreement no. 101093374 and Participating Countries in Project (Czechia, France, Germany, Italy, Slovenia and Spain).


MAX DRIVING THE EXASCALE TRANSITION
SIESTA SCHOOL 2025
17-21/11/2025
Online
Ona Falcó
EuroHPC
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FLEUR

www.flapw.de/MaX-5.1/

FLEUR is an all-electron density functional theory code based on the full-potential linearized augmented plane wave (FLAPW) method. It can be applied to crystalline solids of all chemical compositions in three-dimensional bulk setups as well as in two-dimensional films for the simulation of surface properties. Due to the highly accurate approach, the code is particularly well positioned to describe phenomena on small energy scales, like those arising in complex, non-collinear magnetism or due to spin-orbit physics.

Date: 08-12/05/2023 **Venue:** Jülich (Germany)

All-electron DFT with Fleur:
a Hands-on Tutorial

https://www.cecam.org/workshop-details/1226

The school offered comprehensive training on Density Functional Theory (DFT) and the full-potential linearized augmented-plane-wave (FLAPW) method, with a focus on their practical applications. Designed for researchers and practitioners, the event aimed to enhance participants' understanding of these methods for predicting the electronic, magnetic, and structural properties of materials. Through the sessions, attendees gained advanced insights into the role of DFT and FLAPW in materials screening and development. Additionally, the event fostered valuable interactions between users and developers, promoting collaboration and knowledge exchange. The hands-on part of the school was based on the FLAPW code FLEUR, the GW approximation code FLEUR-Spex, and AiiDA together with the AiiDA-FLEUR plugin.

Applicants: 32 **Participants:** 11 (10M / 1F) **Assessment:** 5.0/5.0

Training material:

Tutorials: https://www.flapw.de/MaX-7.0/tutorial_docker/

Videolectures: https://www.flapw.de/MaX-7.0/video/

Partners: FZJ (DE)

In collaboration with: Psi-k (UK), CECAM (CH)

Organizers: D. Wortmann (FZJ), S. Bluegel (FZJ), and G. Michalicek (FZJ)

Date: 16-20/09/2024 **Venue:** Online

Fleur Hands-on Tutorial 2024

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

The 2024 FLEUR hands-on tutorial offered an interactive learning experience for both new and experienced users of the FLEUR code. Each day featured morning talks on various FLEUR-related topics, followed by hands-on sessions where participants could apply their knowledge, interact with developers, and discuss challenges. The sessions were scheduled at different times to accommodate participants from various time zones. Additionally, a poster session provided an opportunity for participants to present their results and engage with the community.

Applicants: 47 **Participants:** 47 (40M / 7F) **Assessment:** 4.42/5.0

Training material:

Tutorials: https://www.flapw.de/MaX-7.0/tutorial_docker/

Videolectures: https://www.flapw.de/MaX-7.0/video/

Partners: FZJ (DE)

Organizers: D. Wortmann (FZJ), S. Bluegel (FZJ), and G. Michalicek (FZJ)

BigDFT

bigdft.org

The BigDFT suite offers a variety of features, ranging from various ground-state DFT algorithms to potential energy surface exploration techniques. BigDFT uses dual space Gaussian-type norm-conserving pseudopotentials, including those with non-linear core corrections, which deliver all-electron precision on several quantities. Its flexible poisson solver can handle a number of different boundary conditions, including free, wire, surface, and periodic. The code simulates implicit solvents and external electric fields. The code possesses a Linear-Scaling algorithm enabling unbiased DFT simulations of systems up to many thousands of atoms.

BigDFT regularly provides lectures and trainings. Tutorials and lessons are available at: https://l_sim.gitlab.io/bigdft-suite/users/guide.html

Additional resources

Date: 11-15/03/2024 **Venue:** Online

Efficient materials modelling on HPC with QUANTUM ESPRESSO, SIESTA, and YAMBO

https://enccs.se/events/2024-03-efficient-materials-modelling-on-hpc/

In this workshop, participants learned to run common calculations such as SCF, phonons, quasi-particle energies, and time-dependent properties using QUANTUM ESPRESSO, Yambo, and SIESTA. They gained hands-on experience preparing input files and interpreting output files to extract relevant material properties. The program also covered efficient use of HPC resources, focusing on data distribution schemes like plane waves, pools, and images. Participants explored parallelization and acceleration techniques, including MPI, OpenMP, and GPU-offload, as implemented in QUANTUM ESPRESSO, SIESTA, and YAMBO.

Applicants: 118 **Participants:** 78 (53M / 25F) **Assessment:** 4.22/5.0

Training material:

Tutorials: https://enccs.github.io/max-coe-workshop/

Videolectures: https://www.youtube.com/playlist?list=PL2GgjY1xUzfDm9jE90sDPdYeh_B3kj-ij

Partners: SISSA (IT), CNR (IT), ICN2 (ES)

In collaboration with: ENCCS (SE)

Organizers: D. Varsano (CNR) and T. Wikfeldt (ENCCS)

Date: 13-17/05/2024 **Venue:** Ljubljana (Slovenia)

Machine Learning Modalities for Material Science

https://ml4ms.ijs.si/

Machine learning methods are transforming materials design, though they often underutilize data from diverse sources and modalities. This workshop aimed to address this gap by providing young researchers with a comprehensive overview of advanced machine-learning techniques for tackling key challenges in materials discovery. Participants explored strategies for integrating different types of information into a unified framework for materials design. The program featured invited talks, contributed presentations, and panel discussions focused on multi-modal, multi-objective, and multi-fidelity machine learning methods. This interactive format encouraged collaborative thinking and the development of innovative approaches in materials science.

Applicants: 204 **Participants:** 132 (97M / 35F) **Assessment:** 4.62/5.0

Training material:

Videolectures and slides of the presentations are available at: https://ml4ms.ijs.si/recordings/

Partners: IJS (SI), SISSA (IT)

In collaboration with: CECAM (CH), EuroCC SLING

Organizers: S. Džeroski (IJS), S. de Gironcoli (SISSA), P. Rinke (Aalto University), K. Rossi (TU Delft), S. Stevanoska (IJS), and M. Todorovic (University of Turku)

Date: 15-19/04/2024 **Venue:** Trieste (Italy)

Hackathon on mini-app extraction and CI/CD

https://indico.ictp.it/event/10635/overview

This hackathon aimed to develop and enhance mini-apps for testing libraries and components of MaX codes, as well as to reorganize and update the MaX mini-apps repository. During the event, participants defined common output formats and standardized documentation for the mini-apps. Additionally, discussions were held on automating CI/CD processes for the mini-apps across all HPC MaX centres. The hackathon also involved testing and applying protocols for translating Spack recipes to EasyBuild recipes.

Participants: 20 (16M / 4F)

Partners: SISSA (IT), ICN2 (ES), CNR (IT), IJS (SI)

In collaboration with: ICTP (IT)

Organizers: O. Baseggio (SISSA) and the MaX Hackathon Team

Date: 09-13/06/2025 **Venue:** Zadar (Croatia)

School on Machine Learning for Molecules and Materials Research

https://www.cecam.org/workshop-details/school-on-machine-learning-for-molecules-and-materials-research-1379

The school presented modern machine-learning approaches for discovering and designing molecules, materials, and processes. It focused on eight current topics, including high-throughput searches, Bayesian optimization, generative design, and the use of large language models for prediction and potential building. It also covered ML methods for non-adiabatic dynamics, coarse-graining, and integrating experimental data. Lectures gave theory, while tutorials provided hands-on practice. The event fostered collaboration, especially among researchers from widening European countries, strengthened by its setting in Zadar, Croatia.

Applicants: 164 **Participants:** 65 (43M / 22F) **Assessment:** 4.7/5.0

Training material:

Tutorials: https://github.com/rbi-mtm/ml4mmr

Partners: UNIMORE (IT), SISSA (IT)

In collaboration with: CECAM (IT), Psi-K (UK), Cost Action DAEMON, University of Zadar (HR), Ruđer Bošković Institute (HR), Croatian Science Foundation (HR), University Computing Centre Zagreb (HR)

Organizers: K. Batalović (VINCA Institute, University of Belgrade), F. Grasselli (UNIMORE), I. Lončarić (Rudjer Boskovic Institute), J. Ovčar (SISSA), and K. Rossi (TU Delft)

MaX DRIVING THE EXASCALE TRANSITION

PWTK-2024: AN ONLINE TUTORIAL

20-24/05/2024
Online

EuroHPC Co-funded by the European Union

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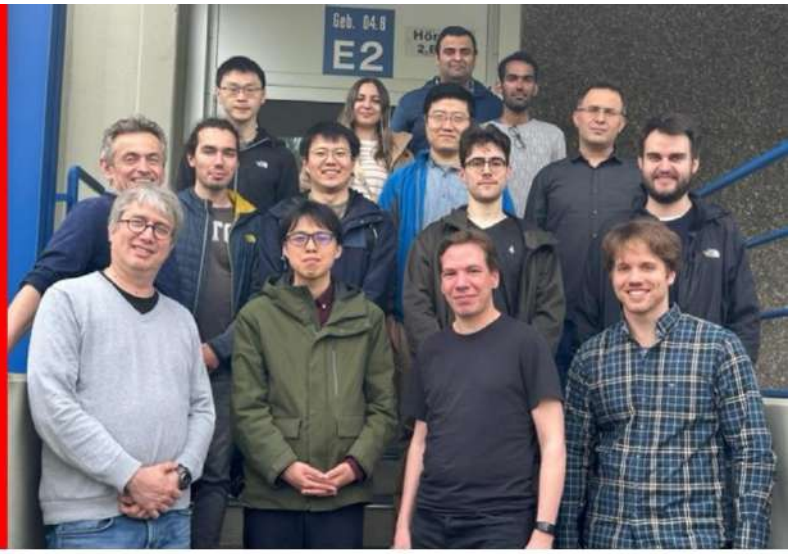
MaX DRIVING THE EXASCALE TRANSITION

ALL-ELECTRON DFT WITH FLEUR

8-12/05/2023
Jülich (Germany)



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MaX DRIVING THE EXASCALE TRANSITION

HACKATHON ON MINI-APP EXTRACTION AND CI/CD

15-19/04/2024
Trieste (Italy)

EuroHPC Co-funded by the European Union

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Participation, diversity, and attendees' satisfaction

Training format and attendance

Between 2023 and 2025, MaX organised a total of **19 training events** aimed at equipping academic and industrial researchers with expertise in MaX codes (**Figure 1**). Of these, **11 were held in person**, allowing participants to engage deeply with expert developers on advanced topics. The remaining **8 events took place online**, enabling broader participation, particularly for introductory-level training. This blended approach proved to be highly effective, as it combined the benefits of in-person learning with the accessibility of virtual sessions. In addition to conventional training, MaX embraced the **hackathon format** by organising **3 events** that offered participants hands-on experience. These hackathons facilitated direct interaction with leading code developers, HPC experts, and industry specialists, creating an environment where learning was driven by collaboration and practical problem-solving.

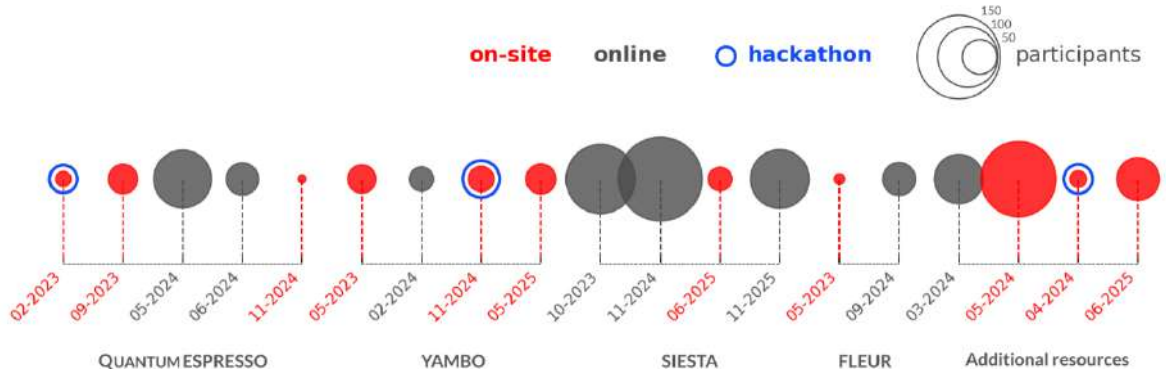

Figure 1: Between 2023-2025, MaX organised 16 training events and 3 hackathons. In particular, 11 events were held in person, and 8 took place online.

Interest, participation, and gender representation

Interest in MaX training has been strong. **Over 2100 researchers applied** to participate, reflecting the high demand for advanced computational training. However, logistical constraints meant that **only 1106 participants could be accommodated (Figure 2)**. **Women made up 27% of participants**, while **female tutors and lecturers accounted for 20%**. MaX recognises the structural gender imbalance in HPC and computational sciences and remains committed to promoting diversity. Efforts continue to increase female participation in event organisation and among invited lecturers, to achieve more balanced representation in future training programs.

Figure 2: Over 2,100 researchers applied for MaX trainings, but logistical constraints limited participation to 1106 attendees. Women comprised 27% of participants and 20% of tutors and lecturers.

Participant demographics

The majority of attendees (75%) came from European countries, while the remaining 25% were from India, the United States, China, and Brazil. Notably, 19% of European participants were from Eastern Europe, reflecting the impact of targeted events in that region (**Figure 3**).

Training satisfaction

Feedback from participants has been overwhelmingly positive. Anonymous evaluations show an **average satisfaction score between "Very Good" and "Excellent"**, highlighting the quality and impact of MaX training events (**Figure 4**). This strong approval underscores the effectiveness of MaX training approach and its commitment to fostering expertise in computational research.

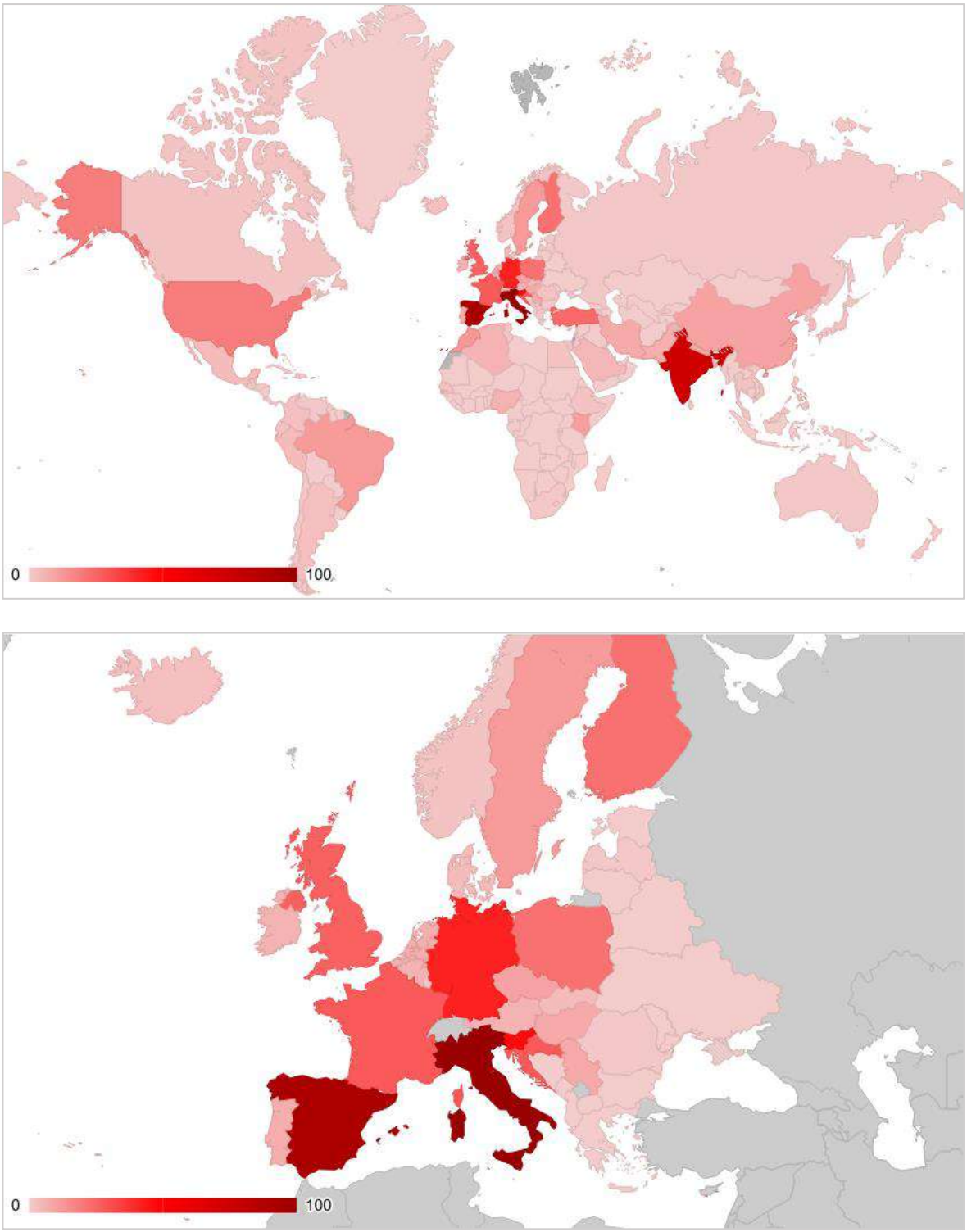

Figure 3: (top) Worldwide and (bottom) European distribution of participants in MaX training events between 2023-2025. The color-scale corresponds to the total number of participants from a given country.

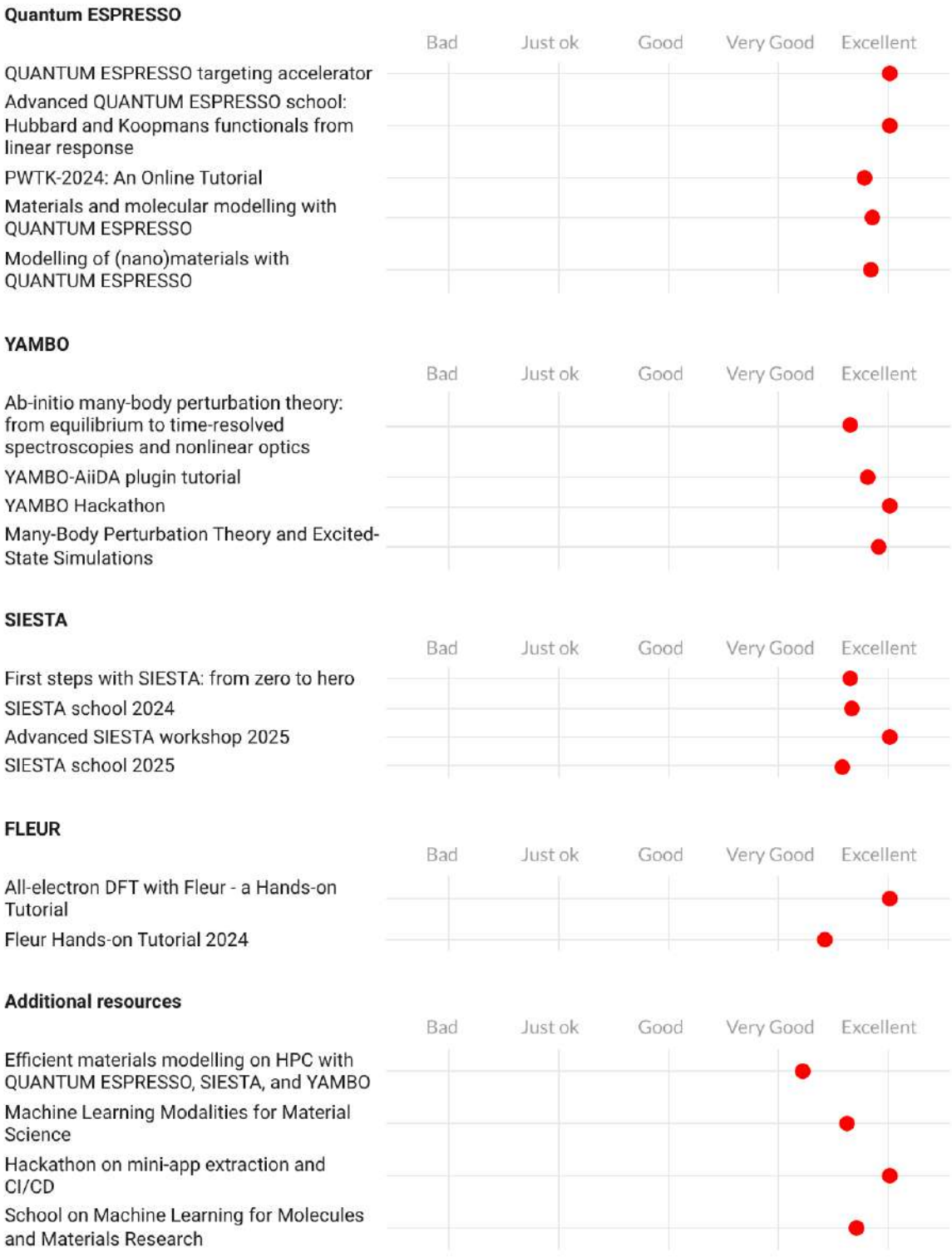

Figure 4: Assessment of MaX training events between 2023-2025, showing a satisfaction score between "Very Good" and "Excellent".

List of Abbreviations

BSC: Barcelona Supercomputing Centre (Spain)

CECAM: Centre Européen de Calcul Atomique et Moléculaire (Switzerland)

CINECA: Consorzio Interuniversitario del Nord-Est per il Calcolo Automatico (Italy)

CNR: Centro Nazionale delle Ricerche (Italy)

CNR-Nano: Centro Nazionale delle Ricerche – Istituto Nanoscienze (Italy)

CSIC: Consejo Superior de Investigaciones Científicas (Spain)

EPFL: École Polytechnique Fédérale de Lausanne (Switzerland)

FZJ: Forschungszentrum Jülich (Germany)

ICN2: Institut Català de Nanociència i Nanotecnologia (Spain)

ICTP: International Centre for Theoretical Physics (Italy)

IJS: Jožef Stefan Institute (Slovenia)

IT4I: IT4Innovations (Czech Republic)

SISSA: Scuola Internazionale Superiore di Studi Avanzati (Italy)

PSI: Paul Scherr Institute (Switzerland)

UNIMORE: Università di Modena e Reggio Emilia (Italy)

NCC: National Competence Centre

CoE: Centre of Excellence

HPC: High-Performance Computing

DFT: Density Functional Theory

BSE: Bethe-Salpeter equation

MBPT: Many-Body Perturbation Theory

NEGF: Non-Equilibrium Green's Function

JU: Joint Undertaking

CI/CD: Continuous Integration/Continuous Development

QE: QUANTUM ESPRESSO

Contact

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For further information regarding past trainings, or to enquire about the organization of a future training, kindly contact Daniele Varsano (daniele.varsano@max-centre.eu) or MaX Management (management@max-centre.eu).

Acknowledgement

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