



DRIVING
THE EXASCALE
TRANSITION

max-centre.eu

MAX codes: webinars, links, facts and figures

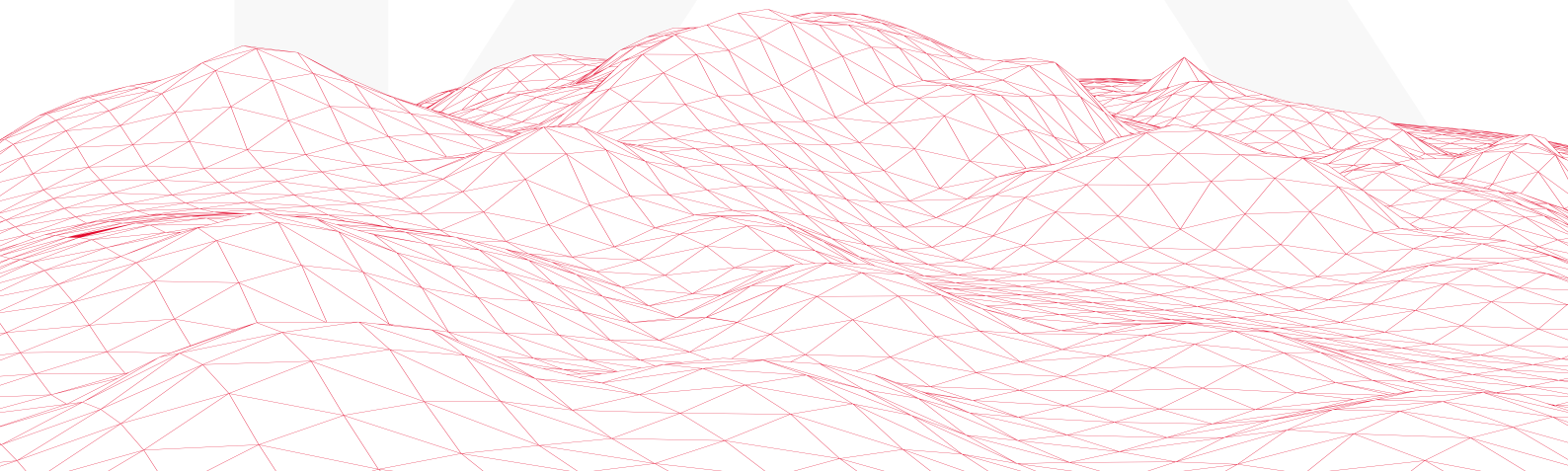


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The webinars series was a collective enterprise of MAX partners.

Editorial editing and content supervision: Maria Celeste Maschio, Maria Bartolacelli, Luisa Neri and MAX Management Team.

Technical and graphical realization: Trust-IT Services.

Introduction

This decade opens with great perspectives for High Performance Computing (HPC), with new architectures allowing sustainable supercomputers working at exascale and beyond. With the opportunities that this scenario offers, computational science also faces new challenges on simulations and data.

The MAX Centre of Excellence, one of the leaders in the field of materials research, is taking up the challenge in redesigning its flagship codes and the data ecosystem in order to take advantage of the new architectures, which are often heterogeneous, and of the new computation and data capabilities.

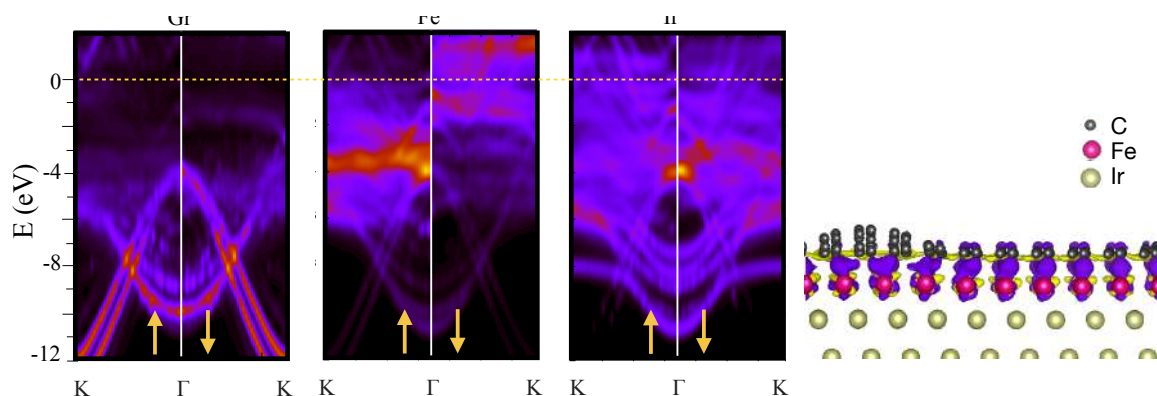
This webinar series was organized in 2020 by MAX to update its users on the novelties introduced in the flagship codes (Quantum ESPRESSO, SIESTA, Yambo, FLEUR, CP2K, BigDFT, AiiDA) which are being ported on these new conceptually different HPC systems.

In this booklet, the successful campaign of 7 webinars is gathered, with a useful collection of the main training materials, contacts and services that MAX offers to its users.

***Elisa Molinari, MAX Director
Cnr Nano and University of Modena and Reggio Emilia, Modena, Italy***

Code overview

[Quantum ESPRESSO](#) is a suite of open-source (GNU GPL) codes for quantum materials modelling using the plane-wave pseudopotential method. The project, started 20 years ago in order to develop a platform for innovative methods for materials simulation and for an easy introduction of numerical algorithms, counts today a world-wide community of outstanding scientific contributors and users. Beside innovation, Quantum ESPRESSO is oriented towards efficiency and aims at ensuring its users a code which is enabled to run on the most novel architectures and technologies.



Band structure of a Gr/Fe/Ir surface, unfolded in the graphene unit cell, and projected in the atomic C, Fe and Ir orbitals and illustration of the atomic structure of the interface. Courtesy of Claudia Cardoso, CNR, Italy

Webinar highlights

The world of HPC is rapidly changing with the advent of alternative architectures that should allow us to build sustainable exaflop supercomputers. Heterogeneous parallelism based on accelerators is currently the most mature of such innovations. New heterogeneous supercomputers are already in the production phase. This webinar was organized to introduce the operation and usage of Quantum ESPRESSO on these conceptually different systems to the Quantum ESPRESSO users. We gave an overview of the actions undertaken by the MAX centre to adapt Quantum ESPRESSO to the new forthcoming architectures. First, the reorganization of Quantum ESPRESSO in different layers: 1) low-level libraries; 2) domain-specific mathematical libraries for performance portability, that - completely encapsulated and provided with functional APIs - can be easily reused in other codes, and for such end, the CoE has made publicly available as part of the MAX library bundle; 3) quantum engine modules, strictly related to QE suite development; 4) applications for property calculators - they comprise the codes interoperating with QE and which users run to obtain their outputs. The second MAX action highlight focused on the CUDA-Fortran porting of Quantum ESPRESSO to systems accelerated with NVidia GPGPUs. The third part of the webinar presented the best practises for the usage and performance optimization of pw.x (the main quantum engine of the suite) on systems accelerated by NVidia GPGPUs.



How to use Quantum ESPRESSO on new GPU based HPC systems

SPEAKERS

Fabio Affinito | **Pietro Delugas** | **Pietro Bonfà**
CINECA | SISSA | Uni Parma & CNR Nano

Facts & Figures

Participants

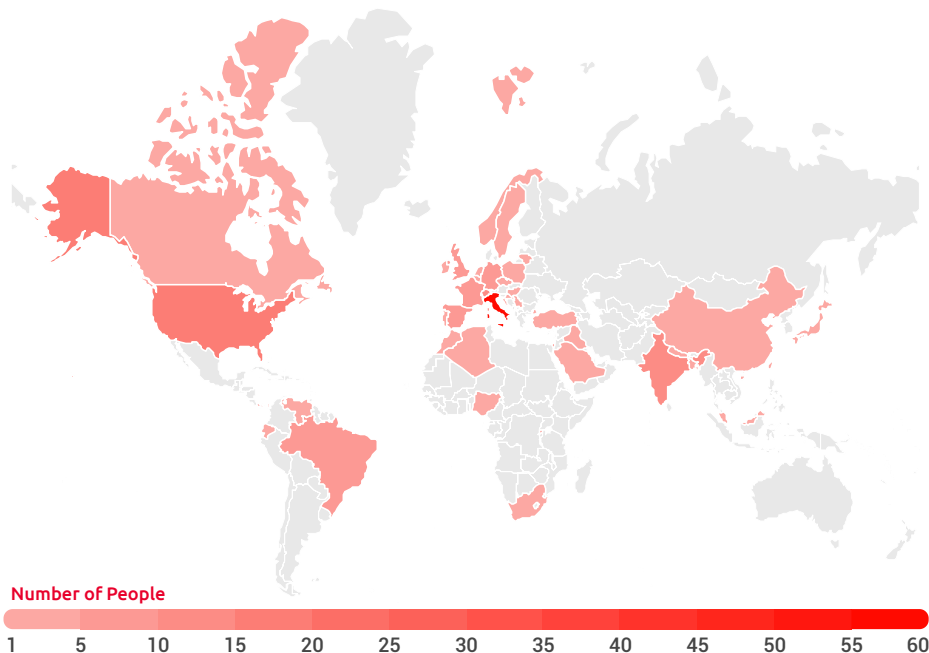
194 Attendees

42 Countries

Gender Balance

78% Men

22% Women

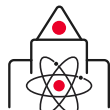


Stakeholders



61%

Research and Academia



22%

Large scale experimental facilities



9%

Industrial and R&D end-users



4%

European & member states institutions



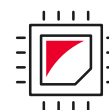
2%

Independent Software Vendors



1%

European HPC ecosystem



1%

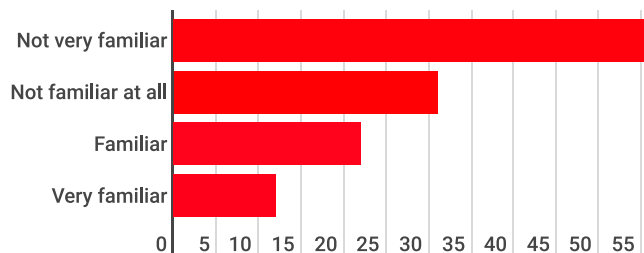
Hardware manufacturers

Poll results coming out of 132 respondents:

Are you a MAX flagship code

52% Yes **48%** No

Are you familiar with GPU based HPC system?



Engagement degree

11 Questions were asked to the speakers

3 Poll-questions (short & immediate)

Almost 98% of the attendees use Quantum ESPRESSO, many of them in combination with Yambo, while 21% performs simulations with CP2K and 16% exploits AiiDA platform. SIESTA is used by 9%, FLEUR by 3% and BigDFT by 2%.

Contacts

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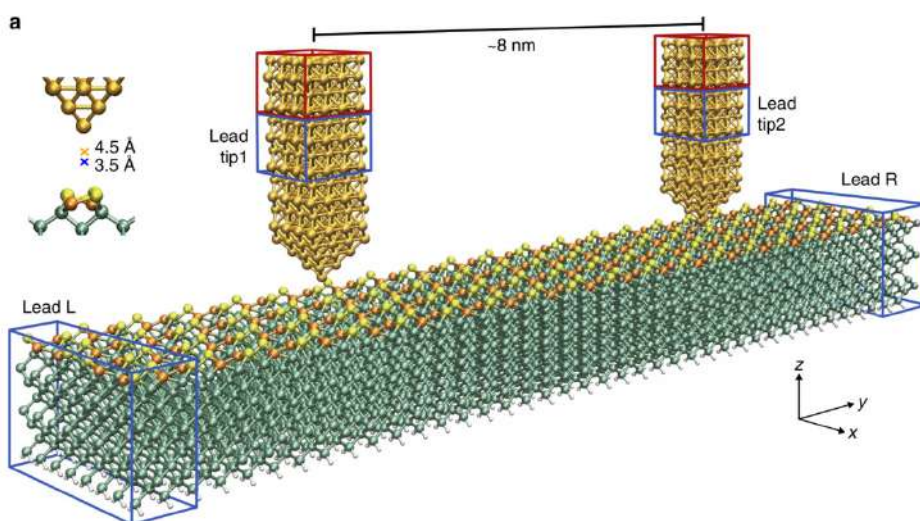


SPEAKERS

Emilio Artacho Univ. of Cambridge and Nanogune	Mónica García-Mota Simune Atomistics SL	Pablo Ordejón ICN2	Nick Papior DTU	Alberto García ICMAB-CSIC
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Code overview

SIESTA is a code based on DFT that has enabled the treatment of large systems with first-principles electronic-structure methods, bringing new opportunities to many disciplines. At the core of SIESTA's efficiency is the use of a basis of strictly-localized atomic orbitals. Systems composed of dozens to hundreds of atoms can be treated with modest hardware, and the programme can employ novel algorithms to handle even larger systems. A very important feature of the code is that its accuracy and cost can be tuned in a wide range, from quick exploratory runs to highly accurate simulations.



First-principles transport simulations for the two-probe experiments. DOI: [10.1063/5.0005077](https://doi.org/10.1063/5.0005077)

Webinar highlights

MAX is preparing materials-simulation codes for the upcoming extreme-scale HPC systems. Within the project, SIESTA's baseline efficiency has been improved, at the same time that the domain of applicability of the code has been expanded with the addition of new features. A very important aspect of these improvements to the usability and performance of the programme is that they are an example of the power of modularization and code reuse, which have been espoused by MAX and by other international initiatives, such as the Electronic Structure Library and the [ELSI project](#). In particular the new developments in the area of electronic structure solvers, notably the incorporation of an interface to the ELSI library, have enabled significant performance enhancements, including GPU acceleration. Another representative area of SIESTA's use domain is ballistic electronic transport: the [TranSIESTA](#) built-in module implements a formalism based on non-equilibrium Green's functions, and lately has been improved in its functionality (adding in particular multi-electrode support) and in its performance. Within the SIESTA ecosystem, many efforts - in collaboration with MAX, CECAM and SIMUNE - have been made in enhancing user support, an area of great relevance in view of the extra complexity that emerges - when considering the variety of novel architectures and features.



[Webinar SIESTA](#)

Additional links

[Latest training event](#)
[SIESTA and MAX](#)
[SIESTA Official Page](#)



DATE **SEP 22 2020** TIME **15.00 (CEST)**

New developments in SIESTA for high-performance materials simulations

SPEAKERS
Emilio Artacho (Univ. of Cambridge and Nanogune), Mónica García-Mota (Simune Atomistics SL), Pablo Ordejón (ICN2), Nick Papior (DTU), Alberto García (ICMAB-CSIC)

Facts & Figures

Participants

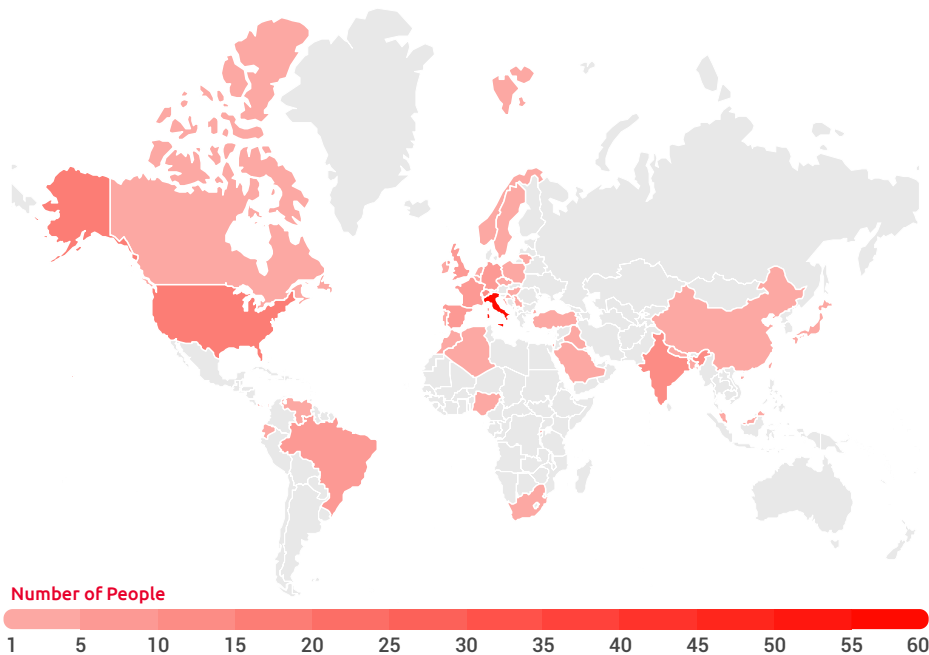
143 Attendees

32 Countries

Gender Balance

76% Men

24% Women



Stakeholders



45%

Research and Academia



32%

European & member states institutions



20%

Industrial and R&D end-users



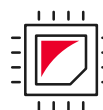
1%

Independent Software Vendors



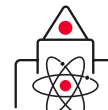
1%

European HPC ecosystem



1%

Hardware manufacturers



0%

Large scale experimental facilities

Poll results coming out to 90 respondents:

Which item has a higher interest for you?

29% Charge analysis

26% Magnetic properties

25% Molecular dynamics

20% Thermal properties

Which of the newly implemented features you find more useful?

31% Hybrid functionals

26% SOC

23% LDA+U

20% TD-DFT

Engagement degree

55 Questions were asked to the speakers

5 Poll-questions (short & immediate)

The attendees run SIESTA on a Linux environment in 90% of cases, on MacOS in 6% and on Windows in 4%. Only 11% used more than 120 CPUs, while 38% employed less than 24 CPUs - the rest uses a variable number of CPUs among 24, 72 and 120. The attendees, in using SIESTA, revealed to be familiar with different tools: ASE (40%), SISL (18%), LUA interface (3%), others (39%).

Contacts

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Quasiparticle Band Structures and Excitons in Novel Materials using the Yambo Code

SPEAKERS

Daniele Varsano
CNR NANO

Andrea Ferretti
CNR NANO

Andrea Marini
CNR ISM

Myrta Grüning
Queen's
University
Belfast

Maurizia Palummo
University
of Rome
Tor Vergata

Code overview

[Yambo](#) is an open-source Fortran code implementing Many-Body Perturbation Theory (MBPT) methods (such as GW and BSE) and TDDFT. It permits the accurate predictions of several electronic and optical properties of condensed matter systems as: band structure of semiconductors, band alignment, defect quasiparticle energies, High Harmonic generation, optics and out-of-equilibrium properties of materials. As input, Yambo requires ground state electronic structure data as computed by density functional theory codes such as Quantum ESPRESSO and Abinit.

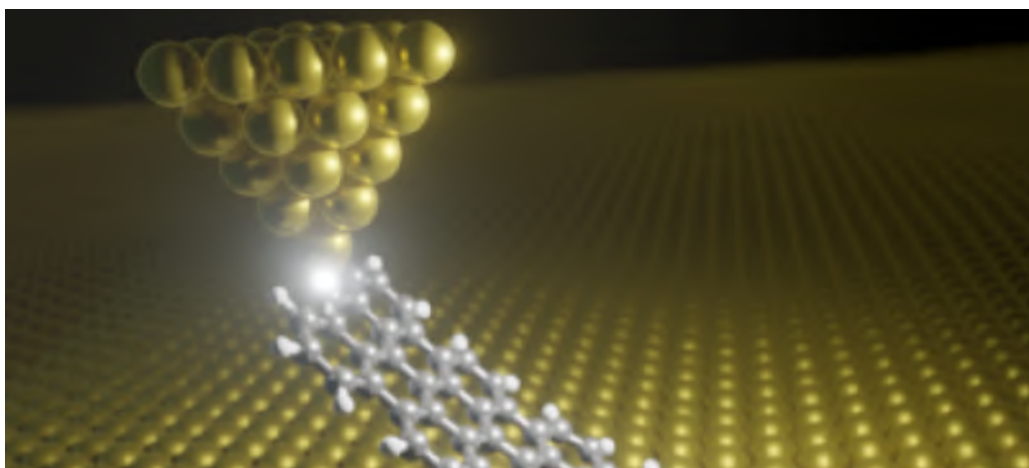


Illustration of "Bright Electroluminescence from Single Graphene Nanoribbon Junctions". Courtesy of Claudia Cardoso, CNR, Italy.

Webinar highlights

New HPC clusters based on accelerators are becoming more and more popular. These machines are conceptually different from most of those previously employed by Yambo users. Indeed, Yambo HPC users are typically accustomed to machines based on massive MPI parallelism, and often need to acquire more familiarity with heterogeneous machines based on GPUs. MAX is preparing Yambo for the forthcoming pre- and exascale machine. As is, MBPT expresses a significant computational complexity and has the potential to exploit new generation architectures, leading to a hierarchy of methods with improving accuracy. Yambo, which has a very highly developed ecosystem in educational and user support, can be used for performing calculations of quasi-particles and excitons (via the GW approximation or the solution of the Bethe Salpeter equation), and also has new advanced features concerning real-time simulations and nonlinear optical spectroscopy. Further developments of the Yambo code involve, e.g., the inclusion of electron-phonon interactions in quasi-particle corrections and optical spectra. [Yambo release 5.0](#) comes with many improvements, novelties, and new features. Among these, it is worth to mention: the extended release of projects for which the gpl version was, so far, limited including the release of new projects contained in the self-consistent module; the reorganization of the executables; an improved command line for the generation of the input files; several improvements to the core part of the code (GW and BSE); and an extended CUDA support.



[Webinar Yambo](#)

Additional links

[Latest training event
Yambo and MAX
Yambo Official Page](#)



Quasiparticle Band Structures and Excitons in Novel Materials using the Yambo Code

SPEAKERS

Daniele Varsano
CNR NANO

Andrea Ferretti
CNR NANO

Andrea Marini
CNR ISM

Myrta Grüning
Queen's University Belfast

Maurizia Palummo
University of Rome Tor Vergata

Facts & Figures

Participants

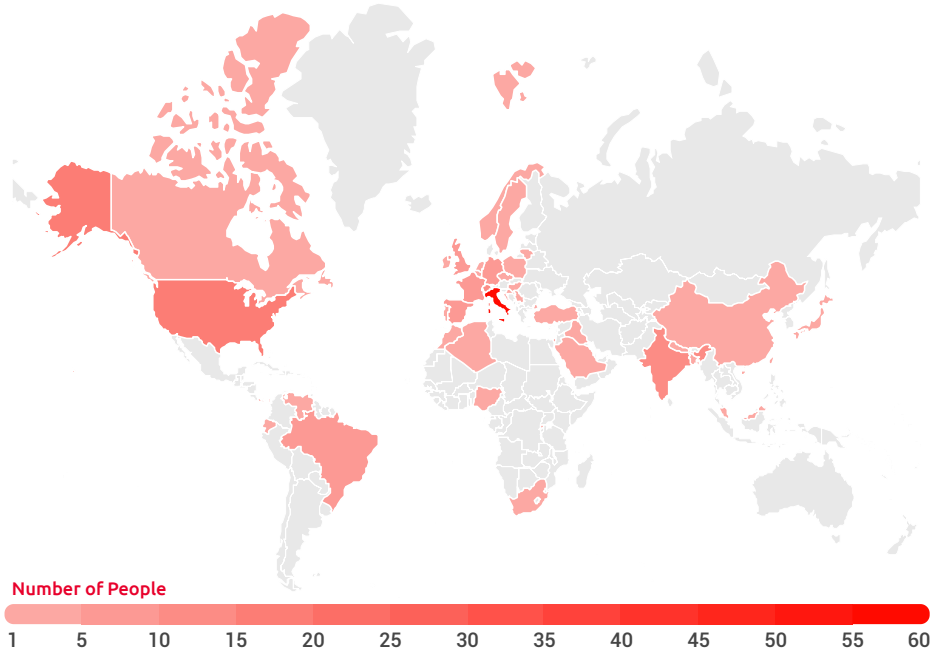
185 Attendees

42 Countries

Gender Balance

76% Men

24% Women

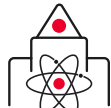


Stakeholders



71%

Research and Academia



17%

Large scale experimental facilities



5%

European & member states institutions



4%

Industrial and R&D end-users



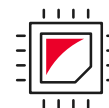
1%

Independent Software Vendors



1%

European HPC ecosystem



1%

Hardware manufacturers

Poll results coming out of 110 respondents:

What is your materials science field?

92% Physics

8% Chemistry

What would you use Yambo for?

61% GW and BSE

17% Mostly GW

13% Real-time optics

9% Other

Engagement degree

7 Questions were asked to the speakers

4 Poll-questions (short & immediate)

Among the attendees, 49% were entry level MBPT users, 42% used it sometime and only 9% were experienced users. Yambo was deployed to study layered materials from 42% of them, bulk systems for 26%, nanostructures for 25% and molecules for 7%.

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All-electron DFT using the FLEUR code

SPEAKERS

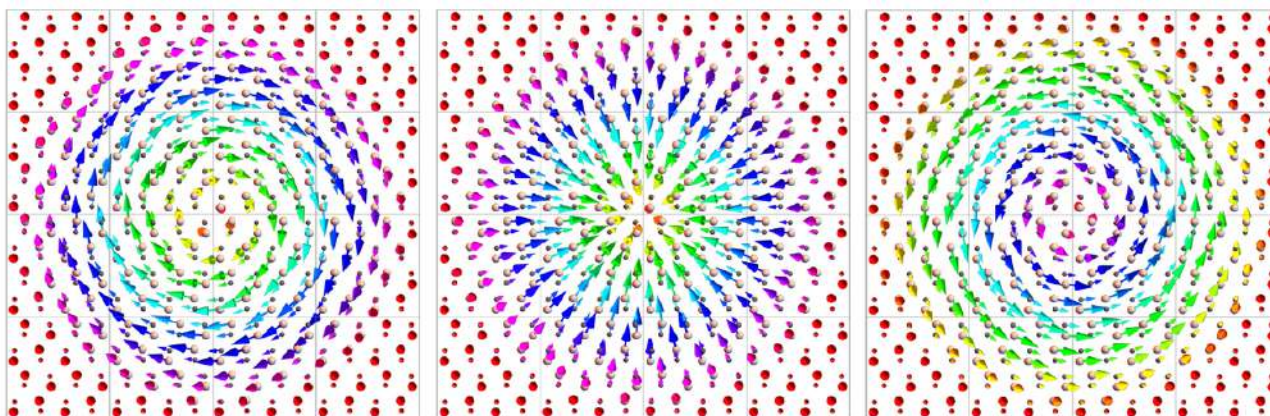
Gregor Michalícek
 Forschungszentrum Jülich

Uliana Alekseeva
 Forschungszentrum Jülich

Daniel Wortmann
 Forschungszentrum Jülich

Code overview

FLEUR is an open source DFT code (MIT license) implementing the all-electron full-potential linearized augmented-plane-wave (FLAPW) method. Its main application is focused on the interplay between the atomic, electronic, and magnetic structures of crystalline solids, surfaces, and thin films. The FLAPW method allows FLEUR users to calculate the XC-functional-dependent DFT answers to material simulation challenges in a controlled way with very high precision. It can be applied without any restrictions on the chemical composition of the material's unit cell and can treat compact as well as open structures with thousands of atoms.



Magnetic Skyrmions in an 8x8x1 MnGe supercell containing 512 atoms. Left and right: Different Bloch Skyrmions. Center: Néel type Skyrmion. Energy decreases from left to right. Courtesy of Uliana Alekseeva and Sergii Grytsiuk, Forschungszentrum Jülich, Germany.

Webinar highlights

The MAX releases of FLEUR represent major evolutionary advances of the code's performance, scalability, and applicability. The ongoing effort to port, adapt, and tune the code to modern HPC architectures pushes the parallelization scaling limits to ever more nodes and thus allows to exploit the capabilities of large compute clusters up to Tier-0 PRACE systems. Even for small-scale parallelizations the introduction of a hybrid MPI+OpenMP parallelization scheme has accelerated the code's execution by a factor larger than 4. As an example usage, it has now become possible to investigate complex magnetic objects like magnetic Skyrmions within a pure DFT description. Interfacing to the AiiDA framework in combination with multi-scale model-based approaches allows to prescreen materials for their capabilities to host such objects. Developer's work on the [MAX 5.0 release of FLEUR](#) has been centered around advanced refactoring, aimed at increasing the usability of the code, separating property calculators from the more computational intensive kernels and incorporating new functionalities. In the future, FLEUR development will be focused on tuning the code to current and future HPC architectures, including more advanced implementations on GPUs (employing OpenACC), stability and interoperability with AiiDA for more complex workflows and enhancing the user's experience.



[Webinar FLEUR](#)

Additional links

[Latest training event
 FLEUR and MAX
 FLEUR Official Page](#)

All-electron DFT using the FLEUR code

SPEAKERS

Gregor Michalicek
Forschungszentrum Jülich

Uliana Alekseeva
Forschungszentrum Jülich

Daniel Wortmann
Forschungszentrum Jülich

Facts & Figures

Participants

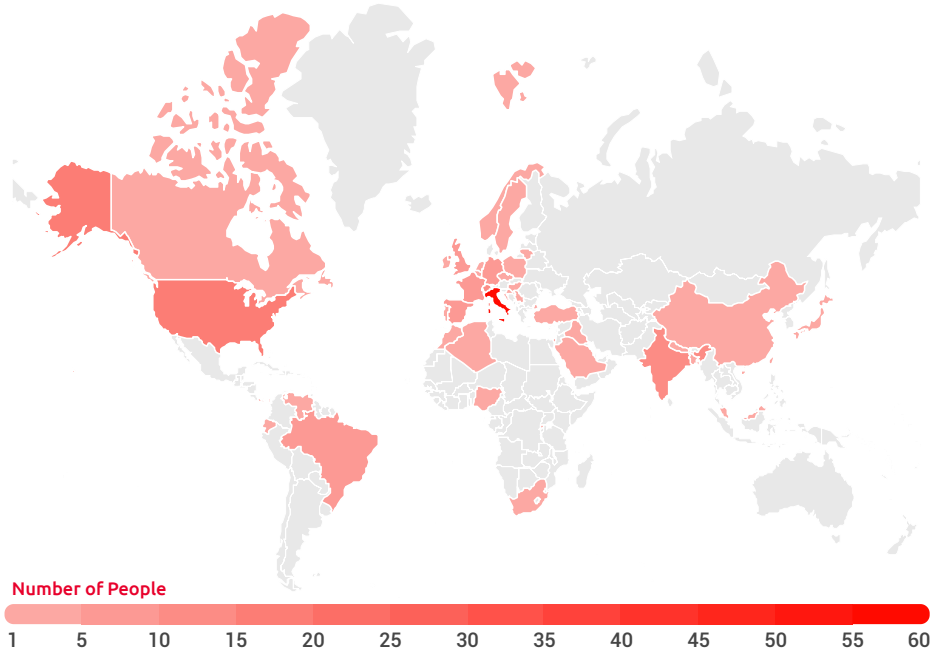
100 Attendees

23 Countries

Gender Balance

77% Men

23% Women



Stakeholders



58%

Research and Academia



23%

Industrial and R&D end-users



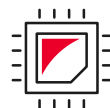
15%

European & member states institutions



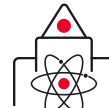
3%

European HPC ecosystem



1%

Hardware manufacturers



0%

Large scale experimental facilities



0%

Independent Software Vendors

Poll results coming out of 81 respondents:

What architecture do you use for DFT calculations?

68% Intel

16% AMD

14% GPU

2% IBM Power

On which computing systems do you perform DFT calculations?

39% Up to Tier-0 supercomputers

37% Up to small compute clusters

20% Notebook and Desktop

4% None at all

Engagement degree

17 Questions were asked to the speakers

3 Poll-questions (short & immediate)

The attendees of this webinar had various backgrounds in DFT: 34% used FLEUR to perform their calculations, 44% relied on other DFT codes, 13% used DFT codes for all-electron calculations while only 9% had no background knowledge.

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gregor.michalicek@max-centre.eu



DATE
JUN 24
2020

TIME
11.00
(CEST)

HPC libraries for **CP2K** and other electronic structure codes

SPEAKERS

Anton Kozhevnikov
ETH Zürich CSCS

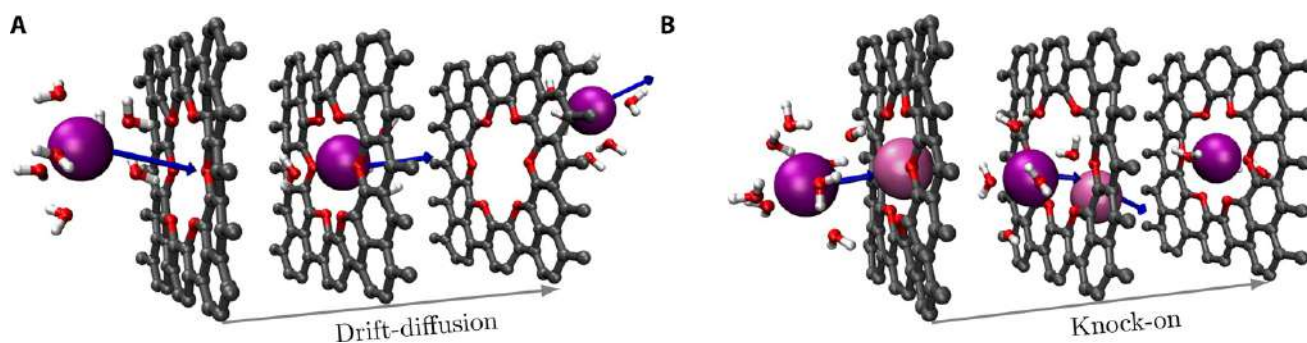
Shoshana Jakobovits
CSCS

Simon Frasch
CSCS

Marko Kabic
CSCS

Code overview

CP2K is a quantum chemistry and solid state physics software package that can perform atomistic simulations of solid state, liquid, molecular, periodic, crystal, and biological systems. CP2K provides a general framework for different modeling methods such as DFT using the mixed Gaussian and plane waves approaches GPW and GAPW. Among the many, CP2K can do simulations of MD, metadynamics, Monte Carlo, and transition state optimization using NEB.



Potential transport mechanisms in graphene crown ether pores. DOI:[10.1126/sciadv.aaw5478](https://doi.org/10.1126/sciadv.aaw5478)

Webinar highlights

CP2K code heavily relies on external libraries for its performance portability as the code itself is written in an agnostic way without any architecture specific implementations. MAX is supporting CSCS in working on HPC libraries which can be adopted by electronic structure codes in order to run them efficiently on current and next-generation hybrid architectures (both NVIDIA and AMD): **DBC**SR is a library designed to efficiently perform sparse matrix-matrix multiplication, among other operations. It is MPI and OpenMP parallel and can exploit NVIDIA and AMD GPUs via CUDA and HIP; **COSMA** is a parallel, high-performance, GPU-accelerated, matrix multiplication algorithm that is communication-optimal for all combinations of matrix dimensions, number of processors and memory sizes, without the need for any parameter tuning; **SpFFT** is a 3D FFT library for sparse frequency domain data written in C++ with support for MPI, OpenMP, CUDA, and ROCm. It was intended for transforms of data with spherical cutoff in frequency domain, as required by some computational materials science codes. For distributed computations, SpFFT uses a slab decomposition in space domain and pencil decomposition in frequency domain; **SIRIUS** is a domain specific library for electronic structure calculations. It implements pseudopotential plane wave (PP-PW) and full potential linearized augmented plane wave (FP-LAPW) methods and is designed for GPU acceleration of popular community codes such as Exciting, Elk and Quantum ESPRESSO.



[Webinar CP2K](#)

Additional links

[CP2K and MAX](#)
[CP2K Official Page](#)



DATE
JUN 24
2020

TIME
11.00
(CEST)

HPC libraries for **CP2K** and other electronic structure codes

SPEAKERS

Anton Kozhevnikov
ETH Zürich CSCS

Shoshana Jakobovits
CSCS

Simon Frasch
CSCS

Marko Kabic
CSCS

Facts & Figures

Participants

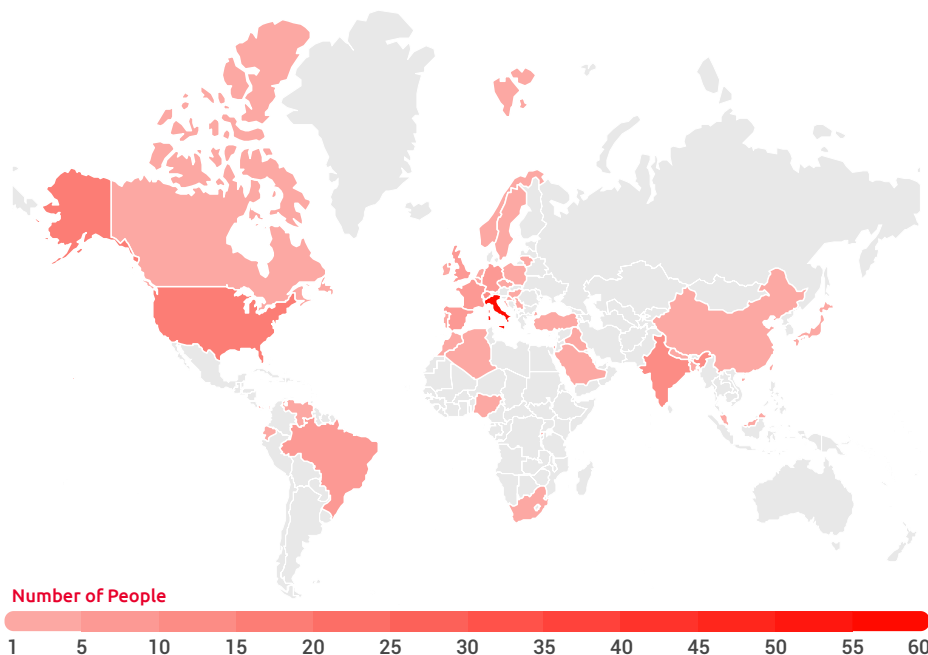
80 Attendees

19 Countries

Gender Balance

81% Men

19% Women



Stakeholders



34%

Research and Academia



22%

Industrial and R&D end-users



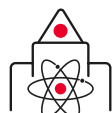
13%

European HPC ecosystem



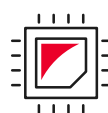
10%

European & member states institutions



10%

Large scale experimental facilities



6%

Hardware manufacturers



5%

Independent Software Vendors

Poll results coming out of 47 respondents:

Do you use GPU-accelerated codes in your research?

39% Yes

32% No

29% Occasionally

What is your priority?

38% Scientific results

36% Both

26% HPC

Engagement degree

21 Questions were asked to the speakers

3 Poll-questions (short & immediate)

Among the attendees of the webinar, only 13% developed usually applications or libraries for GPUs, 19% were occasionally involved in this activities, while 70% were not developers at all.

Contacts

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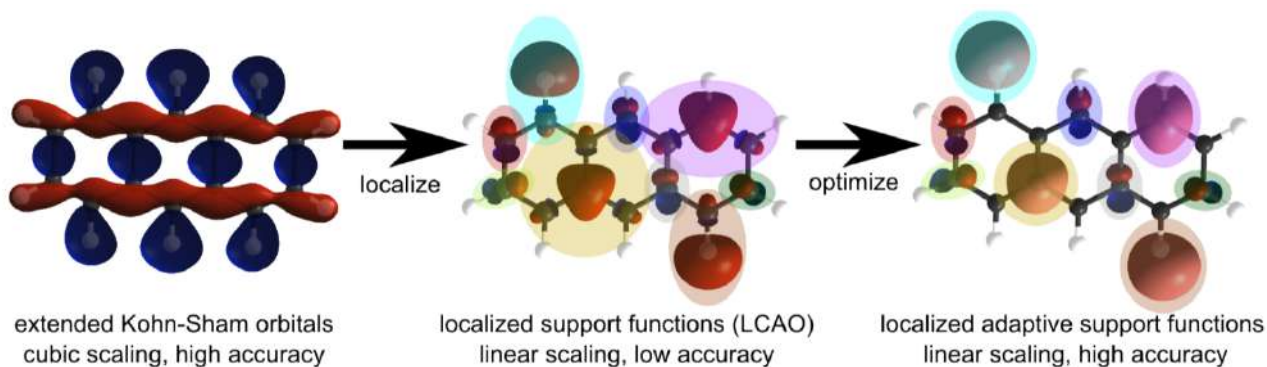
ETH zürich

The Flexibilities of Wavelets for Electronic Structure Calculations in Large Systems

SPEAKERS				
Thierry Deutsch CEA	Laura Ratcliff Imperial College London	William Dawson RIKEN	Augustin Degomme CEA	Luigi Genovese CEA

Code overview

BigDFT is an electronic structure pseudopotential code that employs Daubechies wavelets as a computational basis, designed for usage on massively parallel architectures. It features high-precision cubic-scaling DFT functionalities enabling treatment of molecular, slab-like as well as extended systems, and efficiently supports hardware accelerators such as GPUs since 2009. Also, it features a linear-scaling algorithm that employs adaptive support functions (generalized Wannier orbitals) enabling the treatment of systems of many thousand atoms. The code is developed and released as a software suite made of independent, interoperable components, some of which have already been linked and distributed in other DFT codes.



Schematic illustrating different approaches in BigDFT for the example of anthracene. DOI: [10.1063/5.0004792](https://doi.org/10.1063/5.0004792)

Webinar highlights

In this webinar some examples on the usage of DFT for large-scale systems with BigDFT are reported. It is shown how the localized description of the Kohn-Sham problem, emerging from the features of the basis set, is helpful in providing a simplified description of large-scale electronic structure calculations. MAX enabled the possibility of the implementation of advanced functionalities in the context of pre-exascale computing. [BigDFT 1.9.1 version](#) was released in December 2020. The code has further enhanced its modularity: the compilation of the BigDFT suite is performed via a stacked layer of multiple libraries, most of them being developed outside the BigDFT consortium. BigDFT is an open source code designed for usage on massively parallel architectures. Key features of BigDFT are its high flexibility in simulating complex environments and its innovative numerical approach. Those features find applicability in both molecular and extended systems. The code provides the opportunity to simulate complex materials, to understand information about systems' constituents, allowing for a suitable way of modelling their interaction by reducing the complexity of the simulation. In addition, BigDFT is a MAX code based on wavelets and provides fast, precise and flexible atomistic simulations. In the future, BigDFT will continue to move in the direction of preserving its algorithmic robustness while, at the same time, enabling complex calculation workflow with challenging systems, which would enhance collaboration between different communities.



[WEBINAR BIG DFT](#)

Additional links

[BigDFT Official Page](#)
[BigDFT and MAX](#)

Facts & Figures

Participants

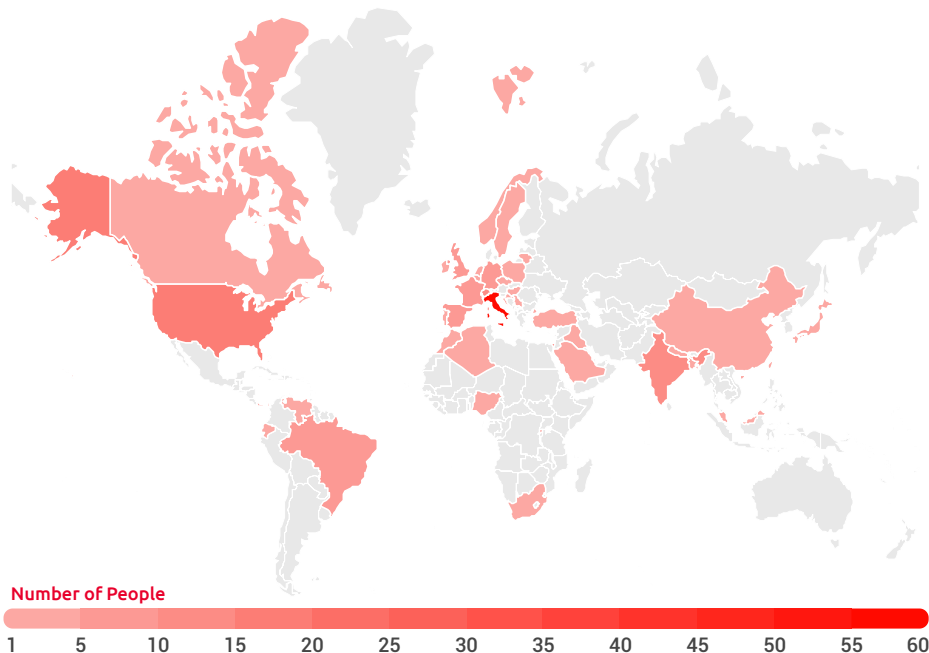
73 Attendees

21 Countries

Gender Balance

86% Men

14% Women



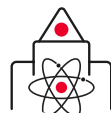
Stakeholders



45%
Research and Academia



26%
Industrial and R&D end-users



14%
Large scale experimental facilities



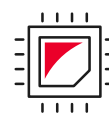
7%
European & member states institutions



4%
European HPC ecosystem



3%
Independent Software Vendors



1%
Hardware manufacturers

Poll results coming out of 38 respondents:

Which are the production calculations, which require any of these features of BigDFT, you are interested in?

- 26%** Large systems and O(N) calculation
- 19%** Flexible boundary conditions (charged systems, electric fields)
- 19%** GPU acceleration
- 17%** Other features available in the code
- 11%** Fragment detection and/or manipulation
- 6%** Implicit solvents
- 2%** None of the above

In which of the following scenarios would you like to use the DFT code for production calculations?

- 42%** I would prefer to run directly on a supercomputer
- 24%** I would prefer to run directly on a laptop/workstation/small cluster
- 21%** I would prefer to adopt a workflow tool on a supercomputer
- 13%** I would prefer to adopt a workflow tool on a laptop/workstation/small cluster

Engagement degree

- 19** Questions were asked to the speakers
- 4** Poll-questions (short & immediate)

The attendees of the webinar were interested in different research topics: surfaces and interfaces (31%), nanomaterials (28%), solids and metals (25%), biological systems (3%), other applications (13%). In general 82% already used BigDFT formalism for their calculations, 11% didn't need the features the code offers, 7% were satisfied with the other codes they already used.

Contacts

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DATE
MAY 27
2020

TIME
15.00
(CEST)

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

SPEAKERS

Sebastiaan Huber
EPFL

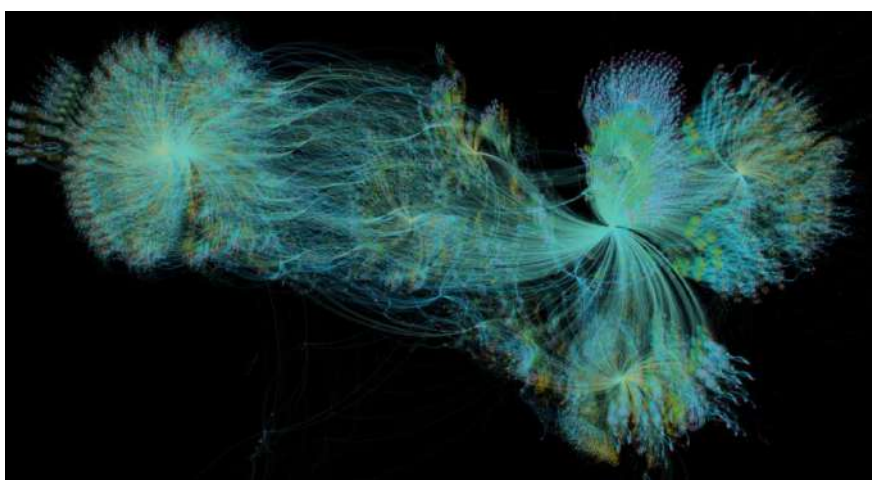
Aliaksandr Yakutovich
EPFL

Valeria Granata
EPFL

Giovanni Pizzi
EPFL

Code overview

[AiiDA](#) (Automated Interactive Infrastructure and Database for computational science) is an open-source Python materials informatics framework to manage, store, share, and disseminate the workload of high-throughput computational efforts. It provides an ecosystem for materials simulations where complex scientific workflows involving different codes and datasets can be seamlessly implemented, automated and shared.



Graphical representation of actual AiiDA database. Courtesy of Jens Broeder, Forschungszentrum Jülich, Germany

Webinar highlights

The available computational power continues to increase, with upcoming supercomputers approaching exascale performance. These advances present great opportunities for computational science, but also pose new challenges on how to automate the simulations and manage the resulting data. [AiiDA](#) is a workflow and data management software, designed to help its users leverage high-performance computing resources to automate workflows of HPC codes, such as those developed by MAX. It allows one to run efficiently high-throughput simulations (HTS) on supercomputers while managing all data produced and ensuring full reproducibility of all results. The 1.x releases of AiiDA come with many performance improvements in the workflow engine and database to support high-throughput computational loads, and many new features to allow users to make optimal use of current and future HPC resources. In addition, the [AiiDALab](#) platform is now available: a cloud GUI solution that makes running these workflows and analyzing the results easy and intuitive, even for non-experts. Finally, the resulting data can be published on the [Materials Cloud Archive](#): an open dissemination platform to publish any data associated with a scientific paper (generated through AiiDA or not), where data is guaranteed to remain online for at least 10 years, and a DOI is assigned to it. Materials Cloud Archive is now recommended as a “stable and recognised open repository in the field of Materials Science” by [Open Research Europe](#) (ORE), the new publishing platform of the European Commission.



[Webinar AiiDA](#)

Additional links

[Latest training event
AiiDA and MAX
AiiDA Official Page](#)



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

SPEAKERS			
Sebastiaan Huber EPFL	Aliaksandr Yakutovich EPFL	Valeria Granata EPFL	Giovanni Pizzi EPFL

Facts & Figures

Participants

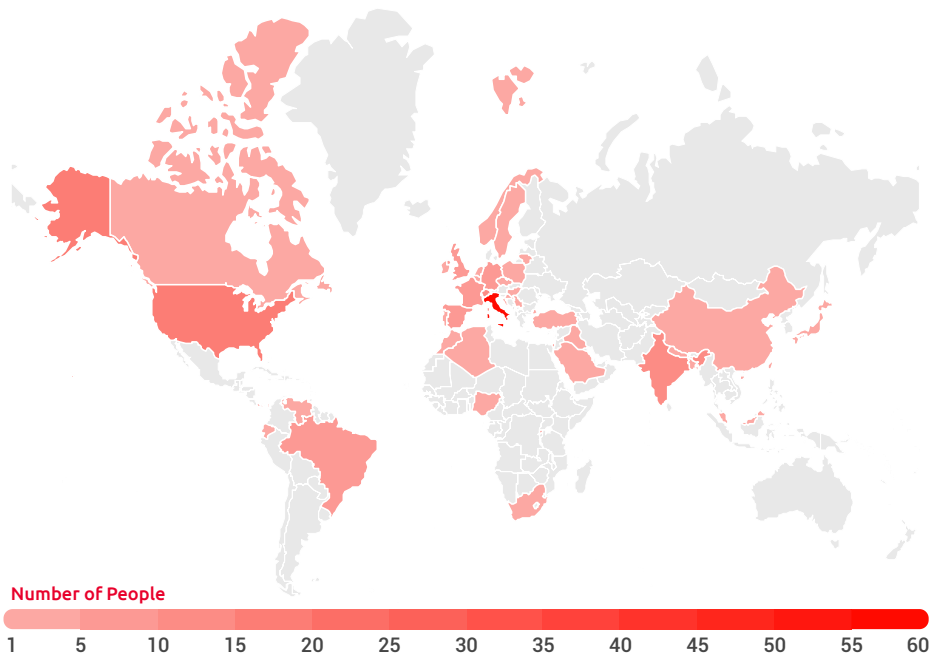
131 Attendees

32 Countries

Gender Balance

79% Men

21% Women



Stakeholders



70%

Research and Academia



12%

European HPC ecosystem



11%

Industrial and R&D end-users



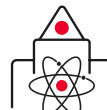
2%

European & member states institutions



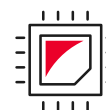
2%

Independent Software Vendors



2%

Large scale experimental facilities



1%

Hardware manufacturers

Poll results coming out of 81 respondents:

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

88% Yes

8% I don't know

4% No

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

81% No **19%** Yes

Engagement degree

6 Questions were asked to the speakers

7 Poll-questions (short & immediate)

Once assessed that 28% of respondents already used AiiDA and that 23% regularly run HTC simulations, it was discovered that 93% thinks that AiiDA is useful for researchers as all of them need to easily reproduce simulations. Nevertheless, 97% never submitted data to the Materials Cloud Archive.

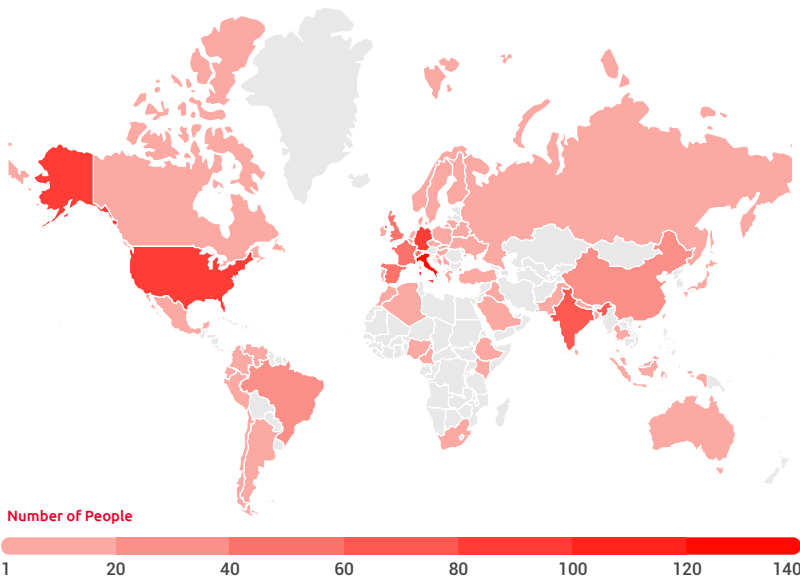
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Below the reader can find a few numbers on the whole webinar campaign. With this booklet our users hold a valuable instrument to know all the effective tools and services that MAX offers in training and support.



Global Numbers

Participants

906 Attendees
66 Countries

Gender Balance

78% Men
22% Women

Stakeholders



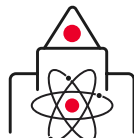
58%

Research and Academia



14%

Industrial and R&D end-users



11%

Large scale experimental facilities



10%

European & member states institutions



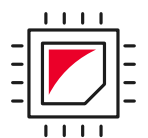
4%

European HPC ecosystem



2%

Independent Software Vendors

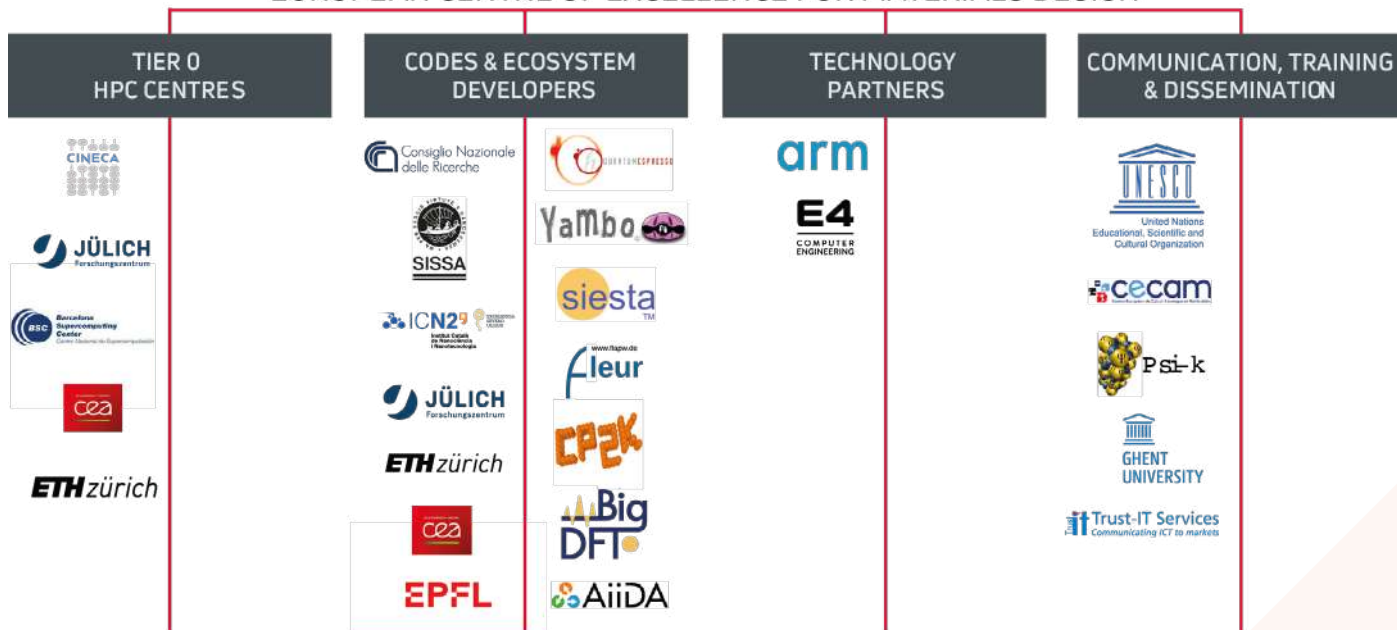


1%

Hardware manufacturers



EUROPEAN CENTRE OF EXCELLENCE FOR MATERIALS DESIGN



MAX coordination and management: Cnr Nano Modena, Italy

Links and Contacts

Science and MAX

www.max-centre.eu/science-and-max/highlights

Training materials

www.max-centre.eu/training-materials

MAX services for users

[Help desk](#)

[High level consultancy](#)

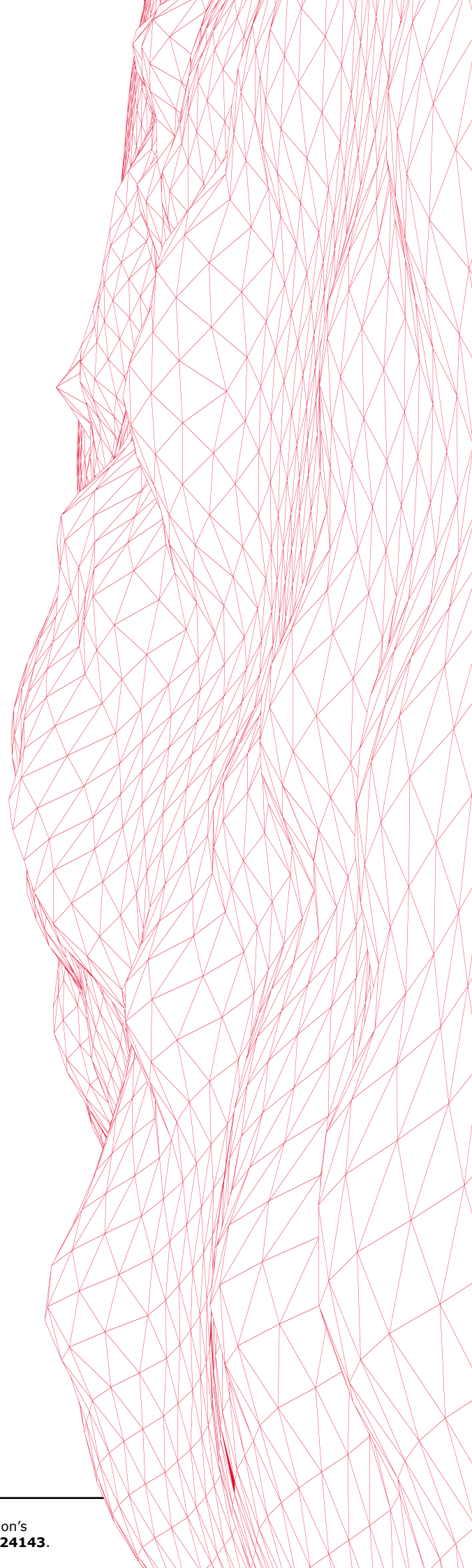
[Turn-key materials solutions](#)

[Container technology for HPC system](#)


[Simulations on premises and in the cloud](#)

MAX flagship codes forums

Quantum ESPRESSO	SIESTA	Yambo	FLEUR	CP2K	BigDFT	AiiDA
User forum users@lists.quantum-espresso.org	User forum siesta-l@uam.es	User forum www.yambo-code.org/forum	User forum http://fleur.xobor.de/	User forum https://www.cp2k.org/howto:forum	User and developers portal https://gitlab.com/l_sim/bigdft-suite/-/issues	User forum aiidausers@googlegroups.com
Bug reporting and other development issues https://gitlab.com/QEF/q-e/-/issues	Development issues https://gitlab.com/siesta-project/siesta/-/issues	Development issues yambo@yambo-code.org	Development issues https://iffgit.fz-juelich.de/fleur/fleur/-/issues	Development issues https://github.com/cp2k/cp2k/issues	Also see https://launchpad.net/bigdft	Registration required, instructions here https://www.aiida.net/mailling-list/



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