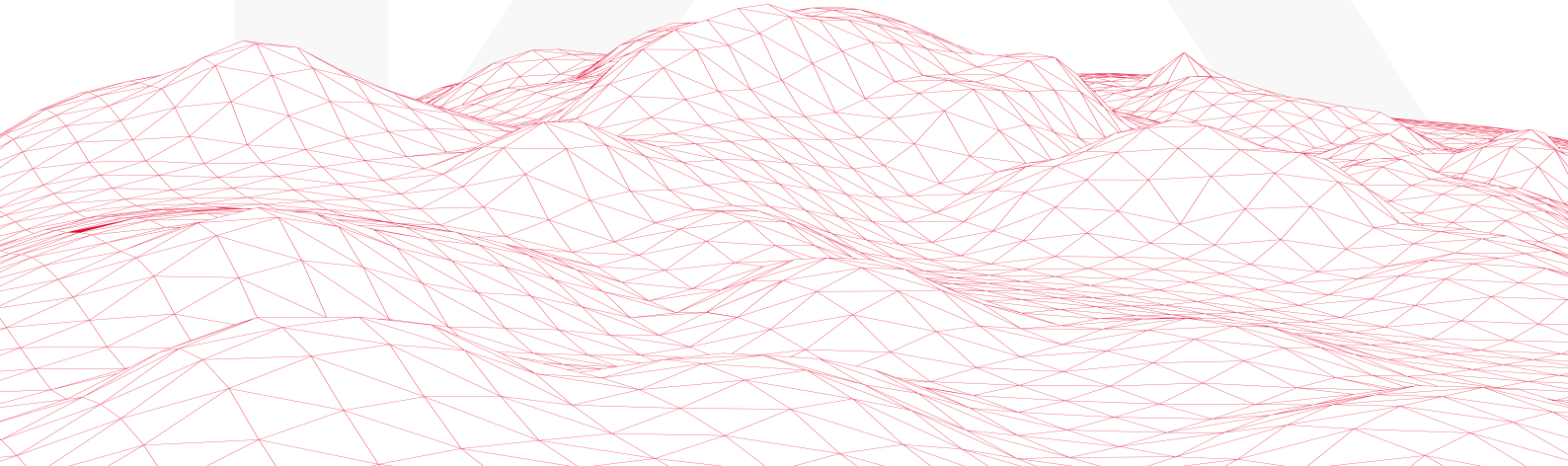
MAX DRIVING THE EXASCALE TRANSITION

max-centre.eu

# MAX codes: webinars, links, facts and figures



# Table of Contents




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***

DATE
**MAY 13**
2020

TIME
**15.00**
(CEST)

# How to use **Quantum ESPRESSO** on new GPU based HPC systems

SPEAKERS

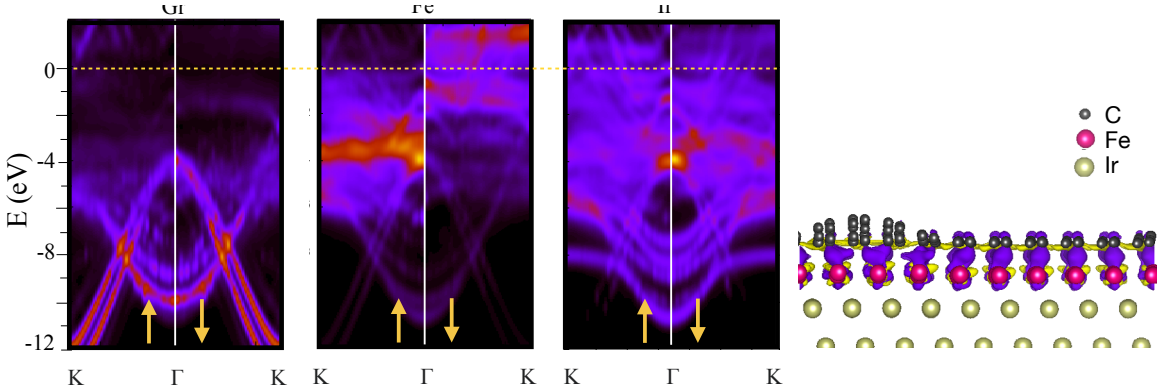
**Fabio Affinito**
CINECA

**Pietro Delugas**
SISSA

**Pietro Bonfà**
Uni Parma & CNR Nano

## 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.

Webinar Quantum ESPRESSO

## Additional links

Latest training event
Quantum ESPRESSO and MAX
Quantum ESPRESSO Official Page

QUANTUMESPRESSO

DATE **MAY 13** 2020

TIME **15.00** (CEST)

# How to use **Quantum ESPRESSO** on new GPU based HPC systems


SPEAKERS

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


# Facts & Figures

## Participants

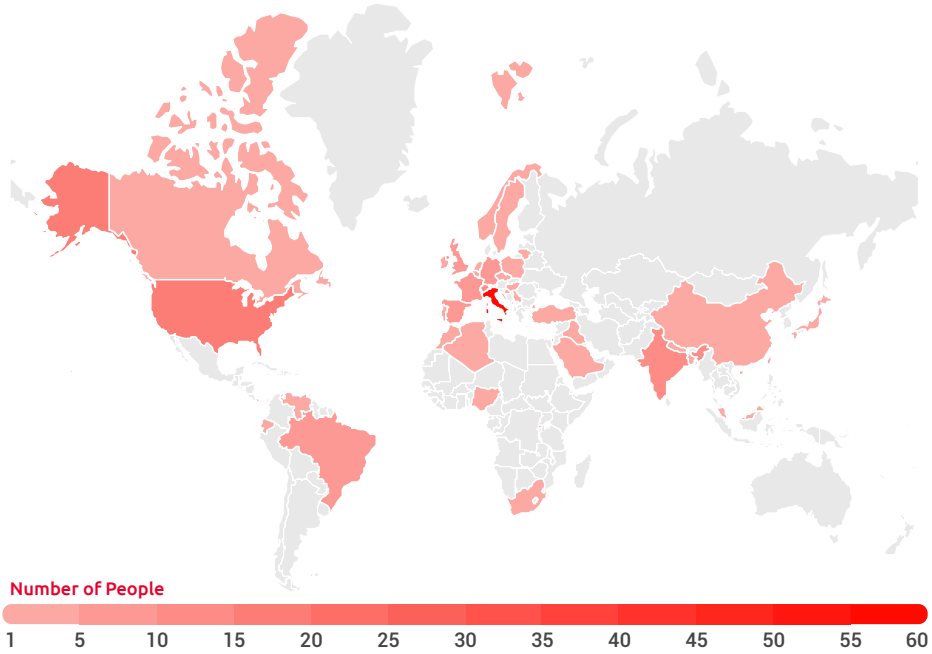
**194** Attendees

**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

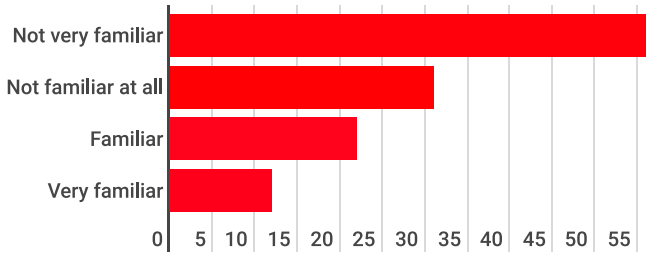
**1%** Hardware manufacturers

## 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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paolo.giannozzi@max-centre.eu

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

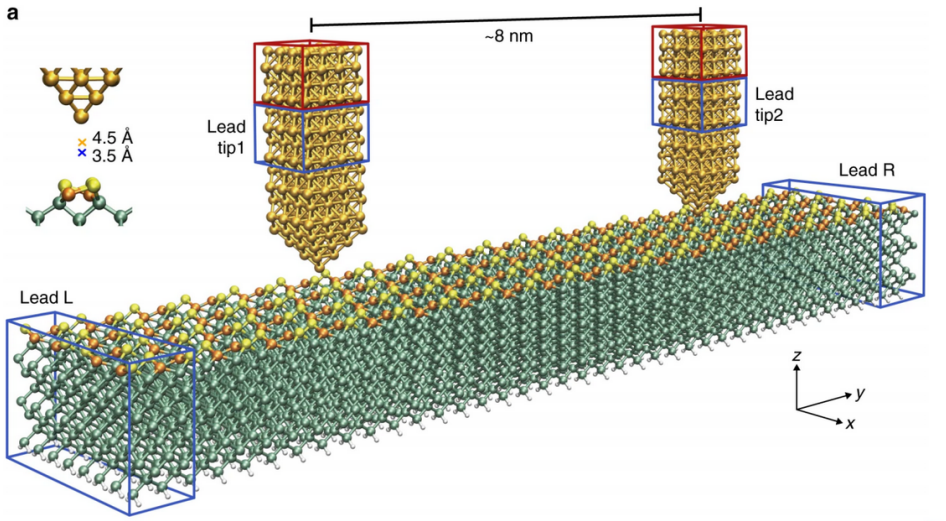
**Pablo Ordejón**
ICN2

**Nick Papior**
DTU

**Alberto García**
ICMAB-CSIC


## 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

## 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

siesta TM

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

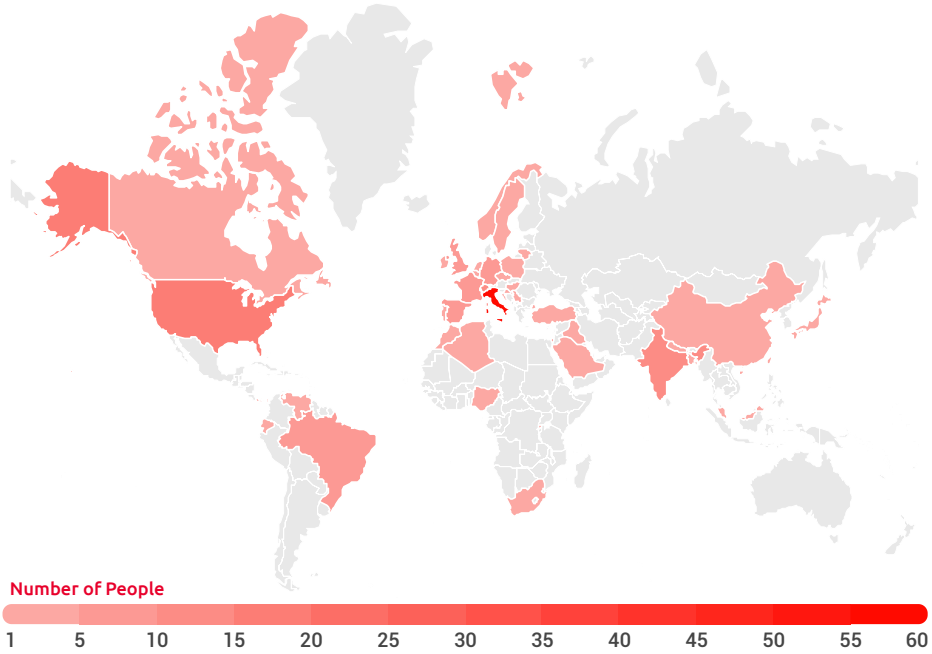
**143** Attendees

**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%).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ICN2 Institut Català de Nanociència i Nanotecnologia

DATE
**JUN 16** 2020

TIME
**15.00** (CEST)

# 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.

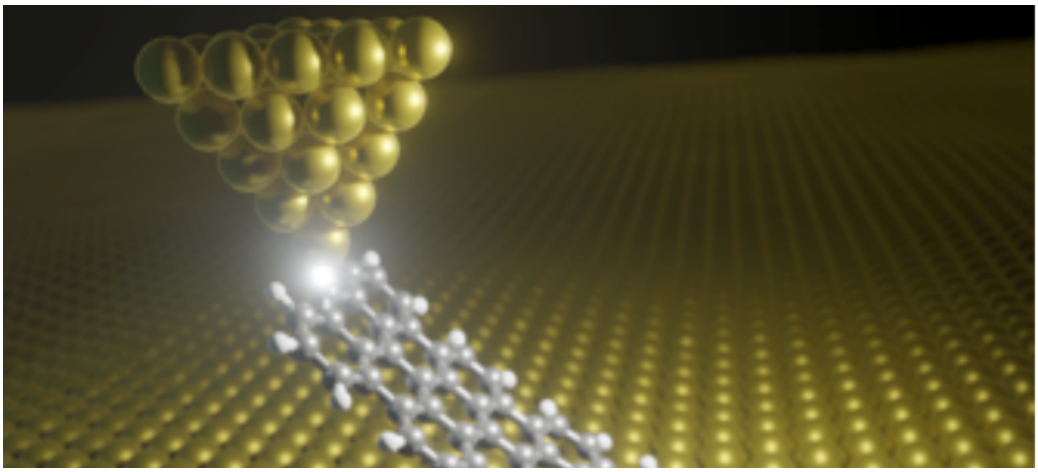


Illustration of "Bright Electroluminescence from Single Graphene Nanoribbon Junctions". Courtesy of Claudia Cardoso, CNR, Italy.

## 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

DATE **JUN 16** 2020

TIME **15.00** (CEST)

# 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

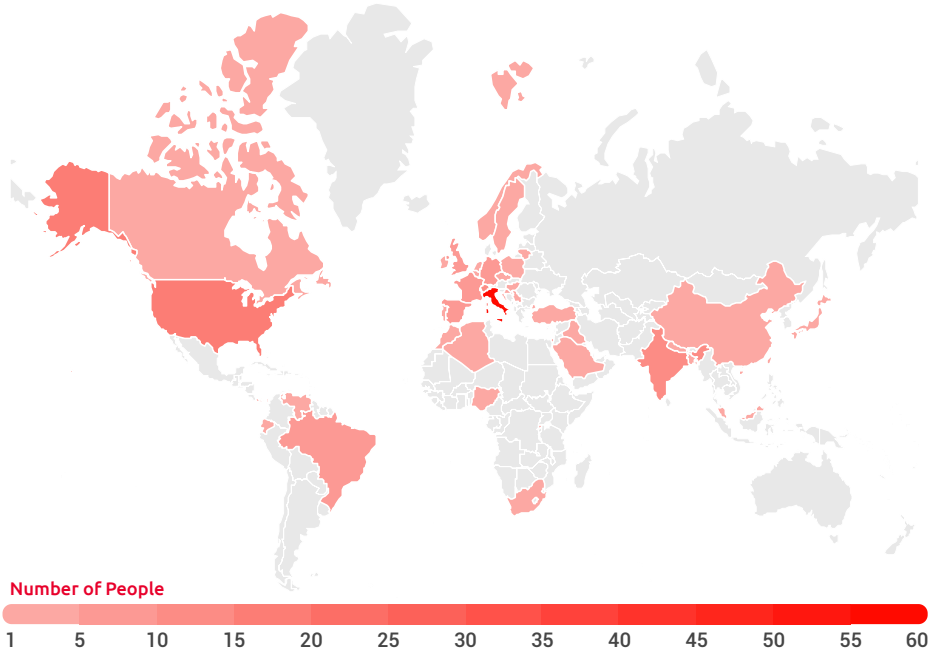
**185** Attendees

**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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Consiglio Nazionale delle Ricerche

www.flapw.de

fleur

DATE
OCT 14
2020

TIME
11.00
(CEST)

# All-electron DFT using the **FLEUR** code

SPEAKERS

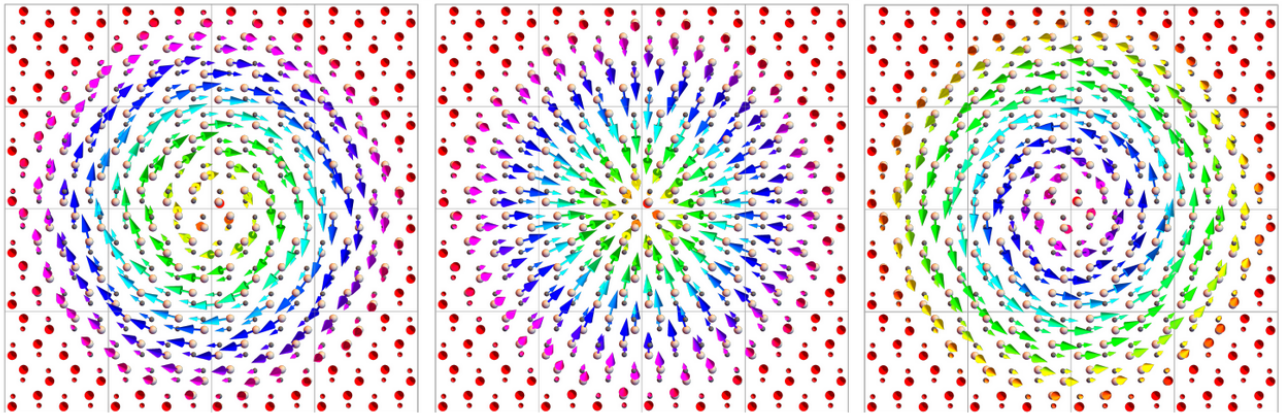

Gregor Michalicek
Forschungszentrum Jülich

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

www.flapw.de

fleur

DATE
OCT 14
2020

TIME
11.00
(CEST)

# All-electron DFT using the **FLEUR** code

SPEAKERS


**Gregor Michalicek**
Forschungszentrum Jülich

**Uliana Alekseeva**
Forschungszentrum Jülich

**Daniel Wortmann**
Forschungszentrum Jülich


## Facts & Figures

### Participants

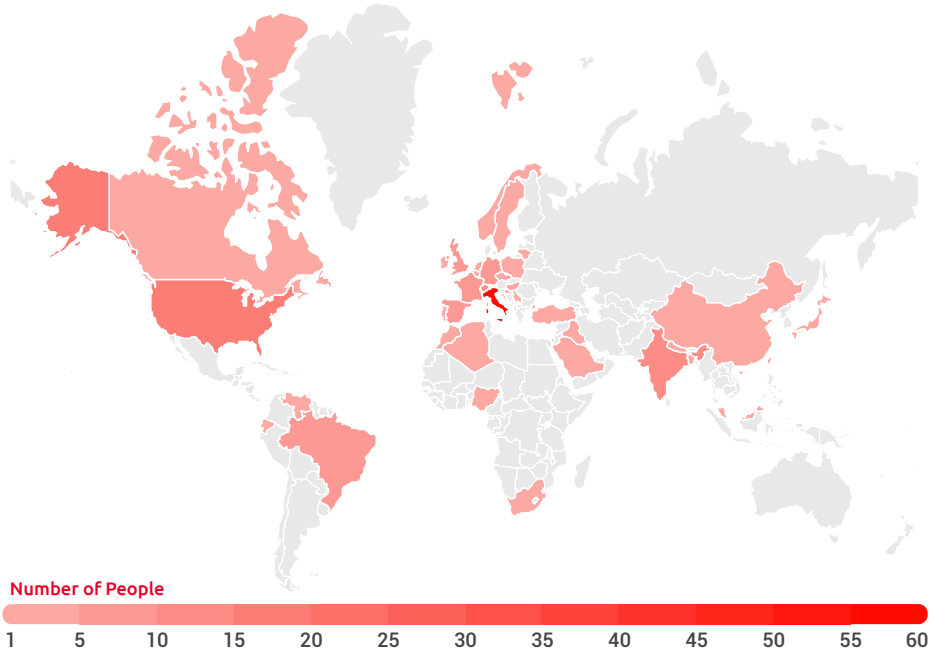
**100** Attendees

**23** Countries

### Gender Balance

**77%** Men

**23%** Women



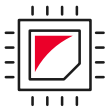

### Stakeholders

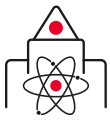

**58%** Research and Academia


**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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JÜLICH Forschungszentrum

DATE
**JUN 24** 2020

TIME
**11.00** (CEST)

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


SPEAKERS

**Anton Kozhevnikov** ETH Zürich CSCS

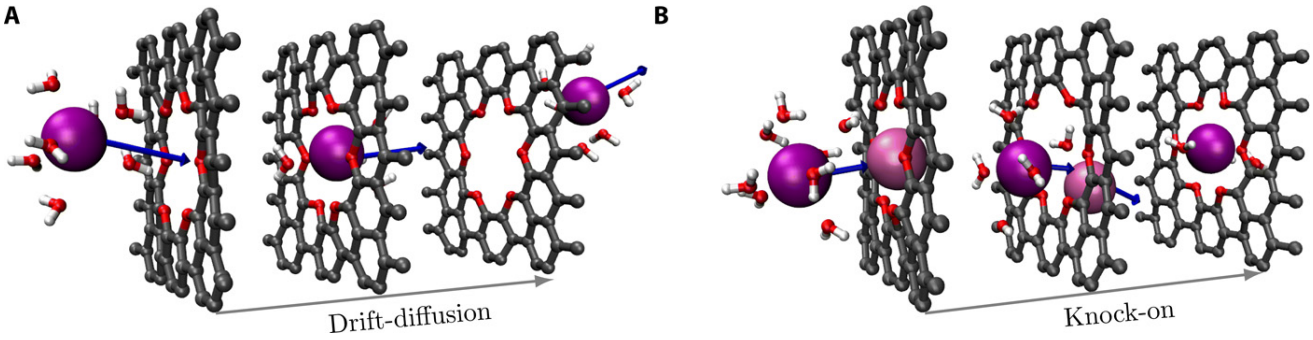
**Shoshana Jakobovits** CSCS

**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

## 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): DBCSR 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

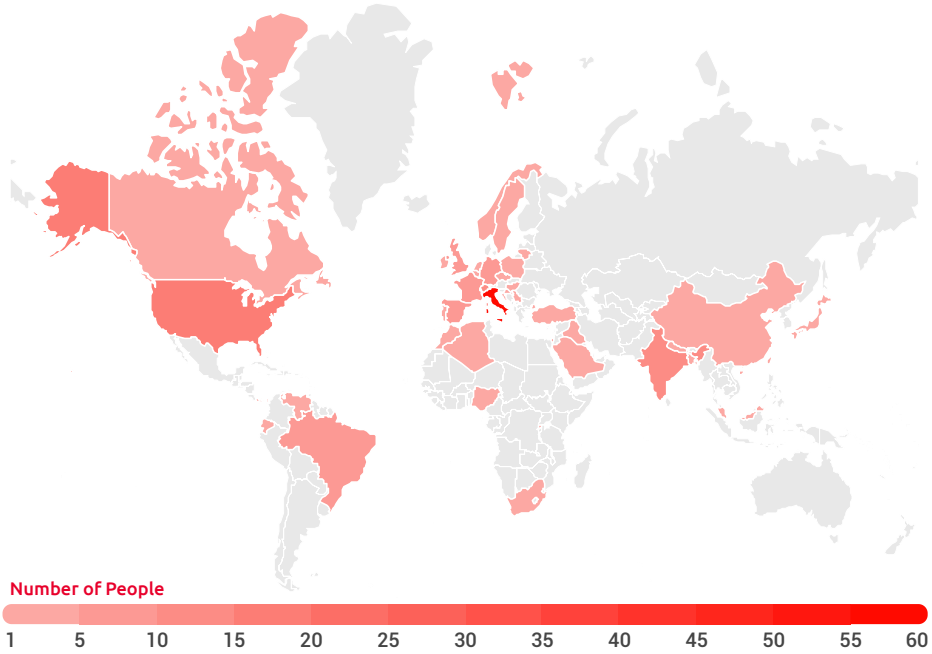
**80** Attendees

**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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anton.kozhevnikov@max-centre.eu


ETH zürich

DATE
NOV 12
2020

TIME
11.00
(CET)

# The Flexibilities of Wavelets for Electronic Structure Calculations in Large Systems


SPEAKERS

Thierry Deutsch
CEA

Laura Ratcliff
Imperial College London

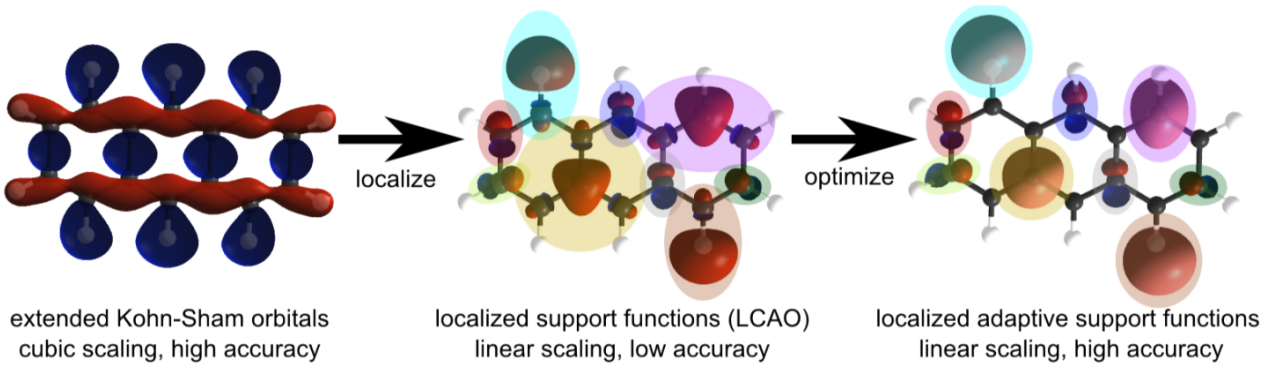
William Dawson
RIKEN

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

## 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

DATE
**NOV 12** 2020

TIME
**11.00** (CET)

# 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

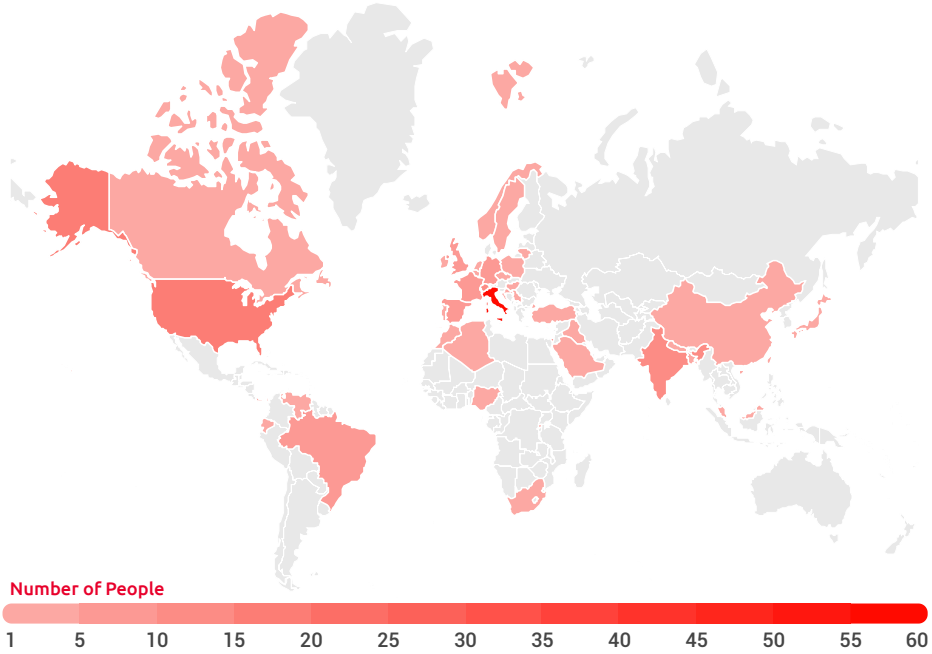
**Luigi Genovese** CEA


## 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 manipulatio

**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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luigi.genovese@max-centre.eu

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

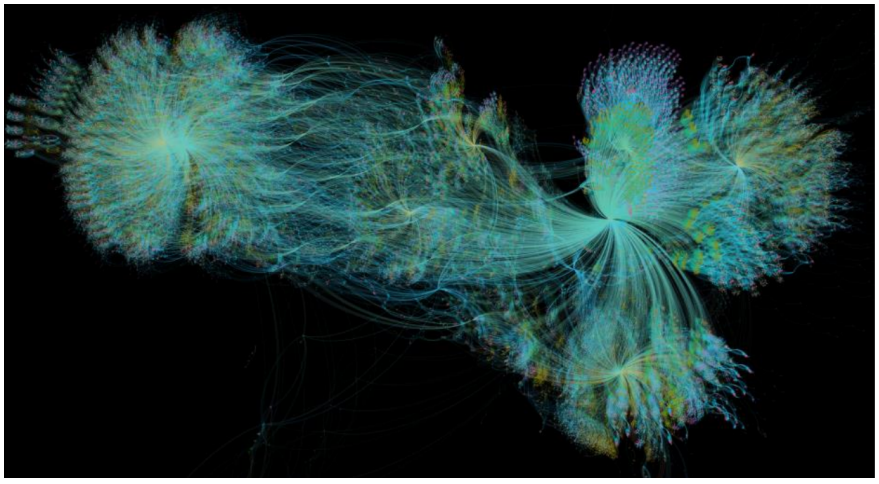
**Aliaksandr Yakutovich**
EPFL

**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

DATE
**MAY 27** 2020

TIME
**15.00** (CEST)

# AiiDA

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


SPEAKERS

| Sebastiaan Huber | Aliaksandr Yakutovich | Valeria Granata | Giovanni Pizzi |
|---|---|---|---|
| EPFL | EPFL | EPFL | EPFL |


## Facts & Figures

### Participants

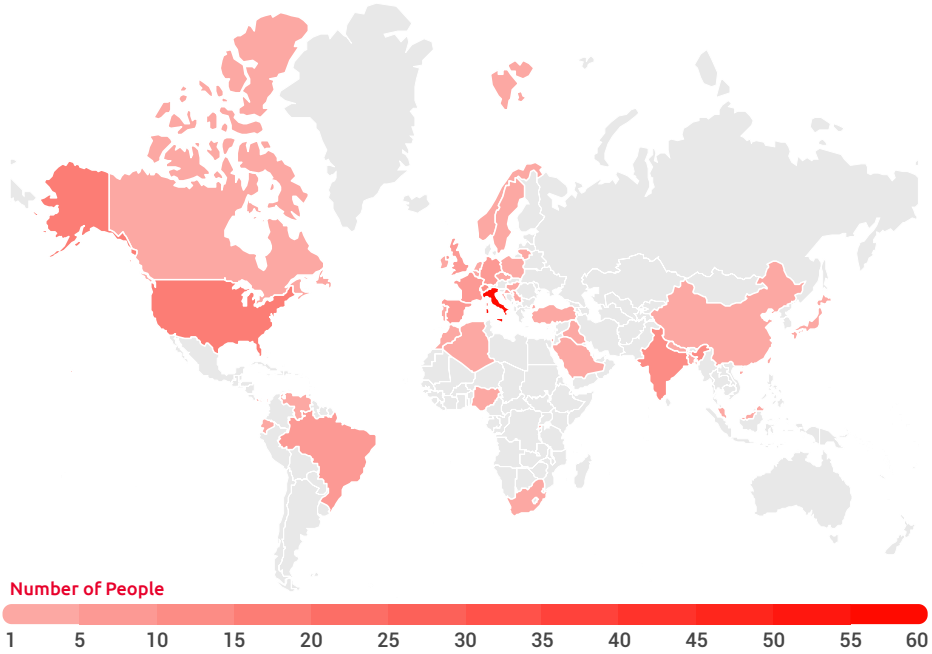
**131** Attendees

**32** Countries

### Gender Balance

**79%** Men

**21%** Women




### Stakeholders


**70%** Research and Academia

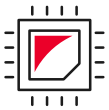

**12%** European HPC ecosystem


**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 date the Materials Cloud Archive.


**Contacts**

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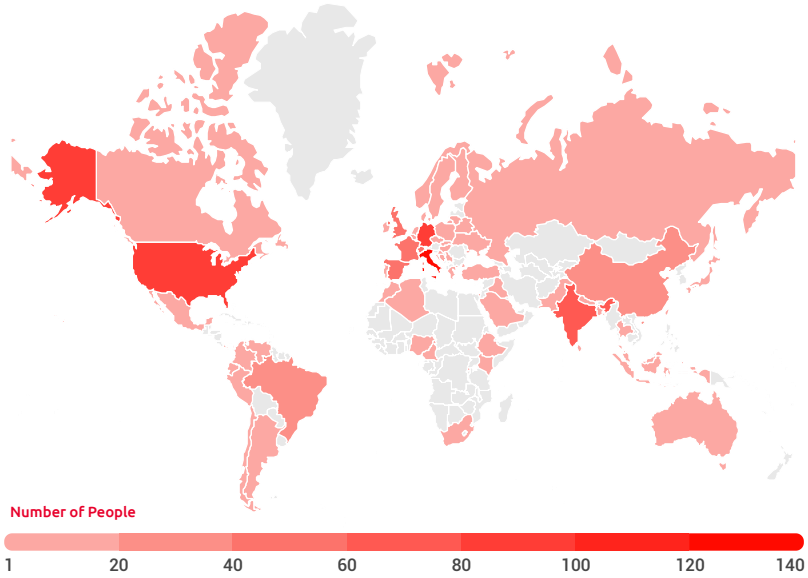
EPFL

MAX DRIVING THE EXASCALE TRANSITION

# Summary

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

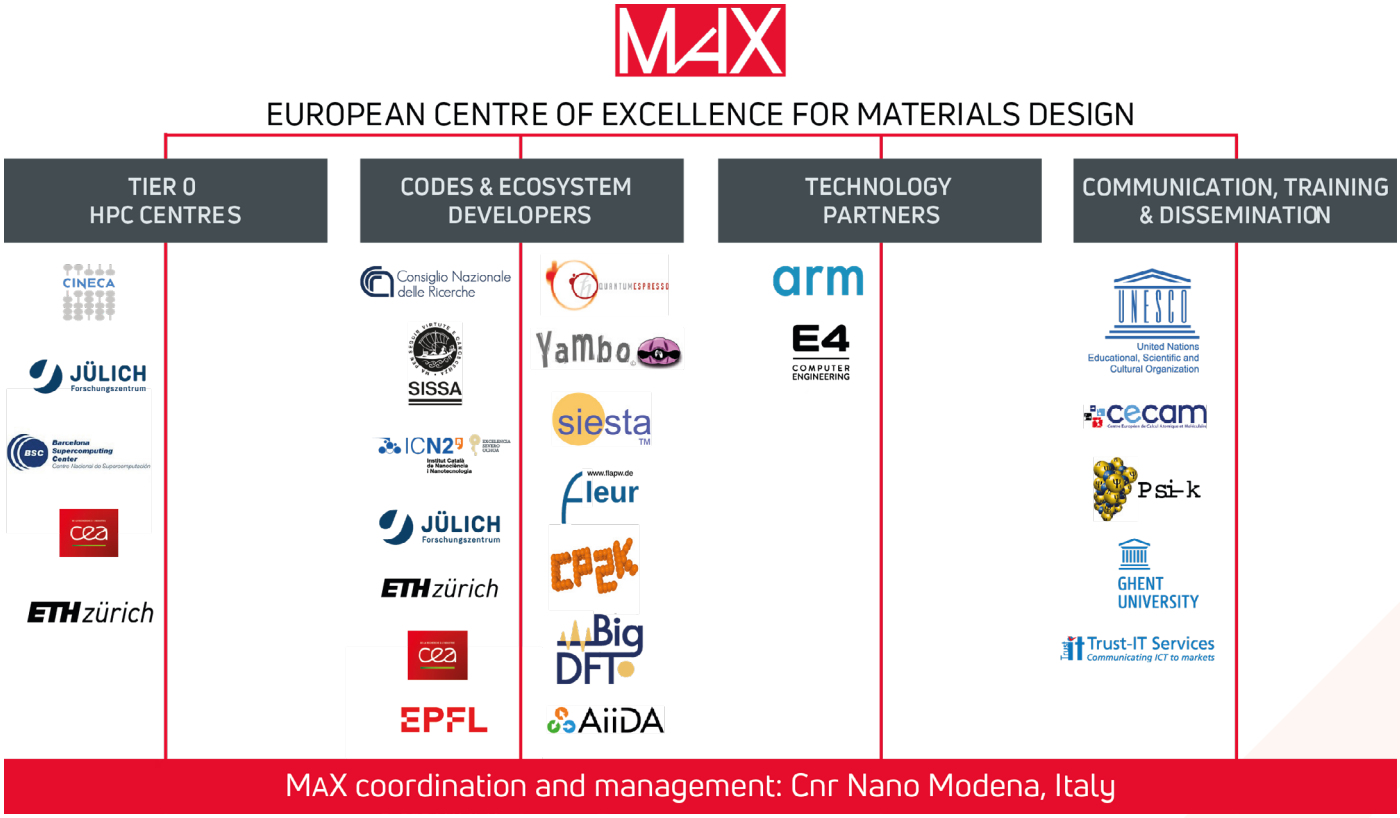
**11%** Large scale experimental facilities

**10%** European & member states institutions

**4%** European HPC ecosystem

**2%** Independent Software Vendors

**1%** Hardware manufacturers



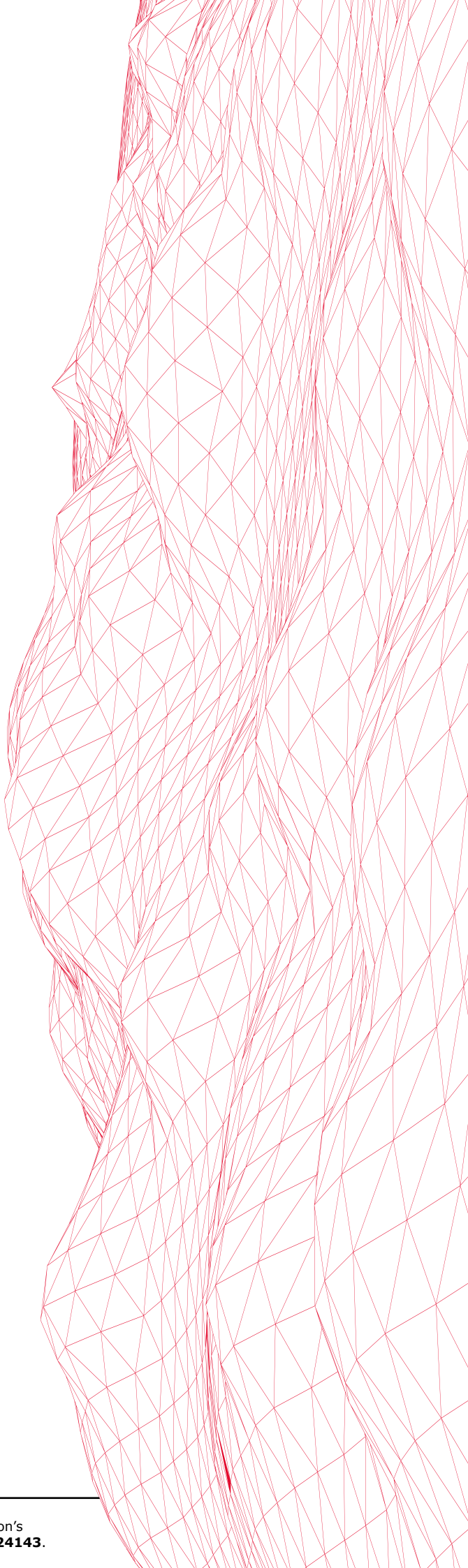

## Links and Contacts

**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/mailing-list/ |



MAX DRIVING THE EXASCALE TRANSITION

**max-centre.eu**

@max_center2

/company/max-centre

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