



SPRING 2016 BOOKLET



DRIVING THE EXASCALE TRANSITION

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Disclaimer.

This booklet contains a brief summary of MaX and its status in April 2016.

It is intended as an informal update and not as a substitute of formal reports and deliverables. Equally informal reports on ongoing tasks in MaX workpackages (WPs) are included in the Annex.

MAX IN A NUTSHELL: WHY, WHAT, WHO, AND HOW

WHY

Materials are crucial to scientific and technological change and industrial competitiveness, as well as to tackle key societal challenges – from energy and the environment to health care, information and communications, industrial processes and manufacturing, safety and transportation. The contribution of High Performance Computing (HPC) to their understanding and design is increasing enormously in recent years, especially in the realm of **quantum** approaches based on electronic structure calculations. In this field, **applications** play a key role and Europe is recognized to be leading in their development. In turn, Materials and Chemical Sciences are now using the most significant share of European HPC resources.

The increasingly high accuracy and predictive power of simulations, combined with higher performance of technologies of computing power and huge leap in storage capacity, is now enabling a paradigm shift in material design and discovery: every increasingly complex material behaviour will be addressed by easily accessible, interdisciplinary, easy-to-use computational experiments. The forthcoming ‘**exascale** transition’ - both in terms of **exaFlops** and **exaBytes**- is expected to allow a major revolution in this domain, making quantum approaches fully viable for complex realistic systems. Quantum materials simulations could heavily enter industrial research and **accelerate** discovery and innovation, similar to what has happened in other domains such as Computational Fluidodynamics or Drug Design.

MaX (Materials design at the eXascale) was born from our conviction that facing the ultrafast evolution of applications that is currently required, and the huge efforts implied in the exascale transition, is **beyond** the capabilities of individual research groups and calls for an **integrated** European initiative. The same is true for the effort to strengthen and expand the **communities** involved in the use and development of quantum materials simulations.

WHAT

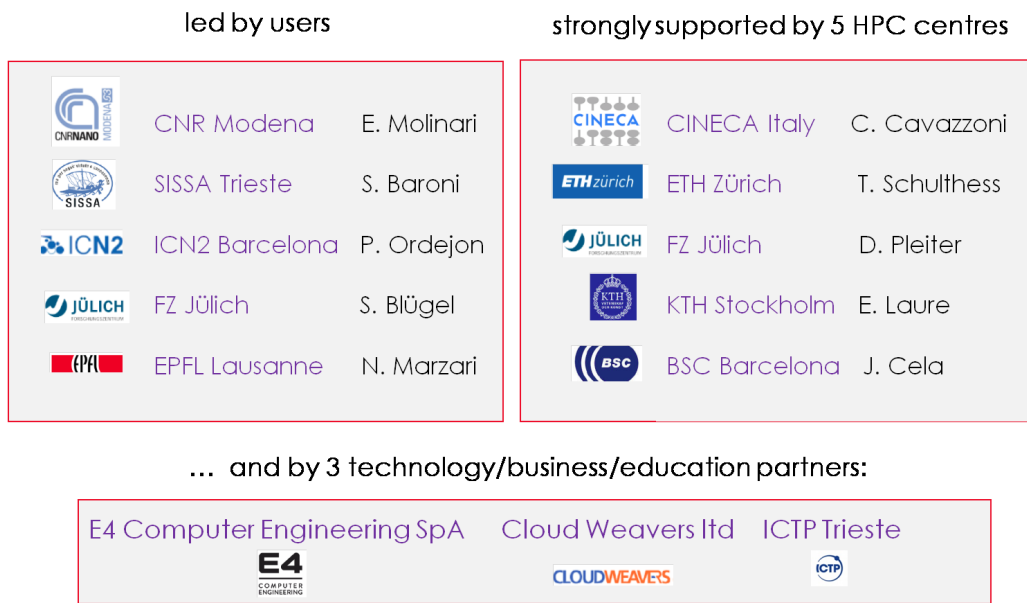
MaX is thus a user-driven European Centre of Excellence established to support developers and end-users in materials simulations, design and discovery. MaX focuses in **enabling the best use and evolution of HPC technologies** by creating and enforcing an ecosystem of knowledge, capabilities, user-oriented services, applications, data workflows, and analytic tools.

At the same time, MaX is **enabling the exascale transition** in the materials domain, by developing advanced programming models, novel algorithms, domain-specific libraries, in-memory data management, technology -transfer and software/hardware co-design actions.

By supporting its advanced quantum materials codes **as recognized reference applications**, MaX is also acting as a pilot center in the wider European effort to advance HPC and data technologies.

WHO

MaX puts together a consortium of 5 research teams, 5 HPC centres, and 3 education and business partners. All together, over 70 researchers are involved in MaX efforts.



MaX is designed and managed to support the needs and the visions of a number of players:

End-users in research and innovation, both in industry and academia, who explore materials discovery and rely on computer experiments.

Domain scientists who develop new methods, algorithms and tools in materials simulations.

Software engineers and vendors who optimise hardware and software performance and usability together with analytical tools for increasingly efficient computer-assisted materials design.

HPC centres, industries and H/W manufactures that are interested in empowering the most advanced and ambitious solutions and in hardware-software co-design.

HOW

The implementation strategy of MaX consists in developing a new application and data ecosystem, and serving its industrial and academic community through end-user oriented actions. MaX key **actions** include:

Implementing a **Sustainable Programming Platform** designed to develop quantum engine kernels and low-level domain specific libraries, to facilitate quantum engines' advanced functionalities and to share libraries with other communities/domains. (This action is mostly developed through WP1.)

Building a **Dynamic Data Framework** to manage the automation of high-throughput calculations, automatic data storage, workflows interchange where data provenance, preservation, reproducibility, and reuse are guaranteed (mostly through WP3).

Supporting a strong action for **Exascale Transition Enabling** through the development of novel algorithms, domain-specific libraries, in-memory data management, and software/hardware co-design (mostly through WP4).

Establishing a **Needs - Solutions Integration** Protocol by aligning the technological offer with leading end-users requirements (mostly through WP2).

Developing a **Catalogue of Services** accommodating end-users help-desk and support, communities' integration, industrial outreach, custom development and consulting (mostly through WP5).

Contributing to the diffusion of material simulations by addressing the skills gap through an integrated offer of **Training and Education** programs in HPC and computational material science (mostly through WP6).

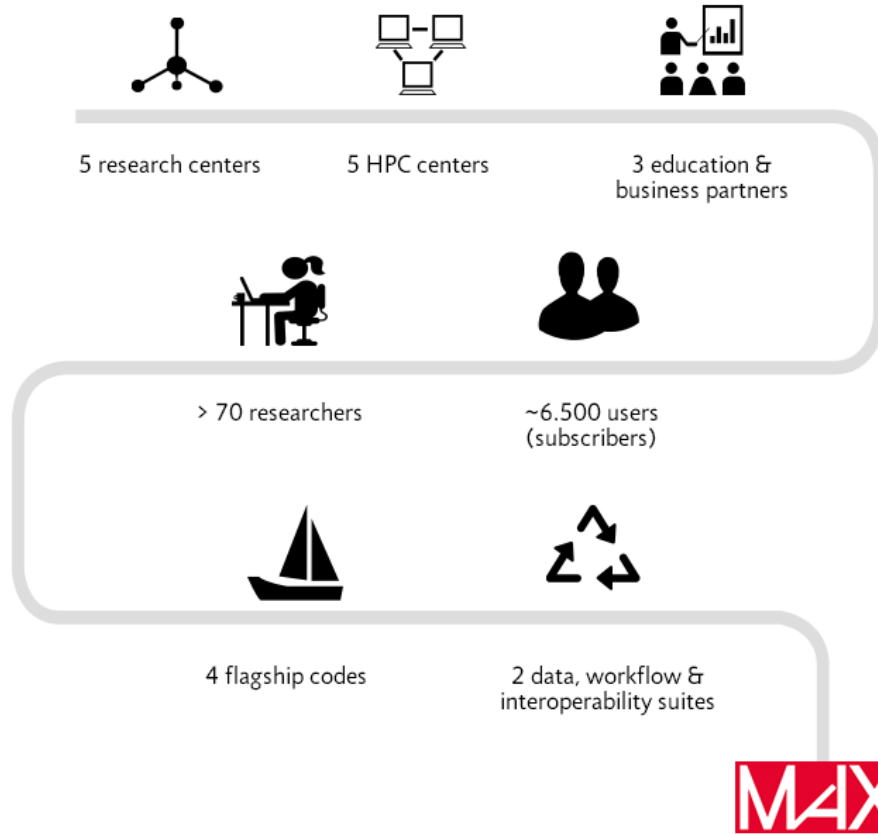
Setting up a Centre working as an **effective e-infrastructure** for its users and for the broader European ecosystem (mostly through WP7).

A number of 'Pilot Cases' are also currently developed in close contact with leading industrial partners representing a challenging test ground for the MaX working approach. The packages and workflows emerging from the Pilot Cases constitute the basis for a '**market-place**', where solutions developed for a given problem will be made available and tailored to other end-users. This opportunity is expected to enable rapid response to shorter-term issues, and could be typically well suited, e.g., for SMEs.

Crucial to this diffusion and scaling-up process is the choice to restrict MaX action to **open-source** codes: this will allow developing and implementing open business models capable of creating value for all the stakeholders.

MaX acts as a central service hub providing coordination and dissemination of the activities, together with process and IT infrastructure management, in the spirit of a Virtual Research Environment and service provisioning. This combined effort and sharing of resources is expected to shift and reduce costs, as well as to act as an outreach multiplier. To guarantee the quality of the provided services MaX maintains toolsets, templates, and documentation of best practices, procedures, and techniques.

MAX IN NUMBERS



ONGOING ACTIVITY (SEPTEMBER 2015–APRIL 2016)



MAX QUANTUM ENGINES: THE FLAGSHIP CODES

WP1-WP2-WP3-WP4-WP5-WP6-WP7

MaX initially focuses on selected flagship codes: widely-used applications, based on rather diverse models, mainly oriented to structural, electronic, magnetic properties and to spectroscopies of materials from first principles: **Quantum Espresso**, **Siesta**, **Fleur**, **Yambo**. A further application, **AiiDA**, is the basic informatics infrastructure adopted and developed for workflows and data management, preservation and sharing.

- MaX is expanding the potential of these flagship codes on the present HPC platforms, by implementing new capabilities and algorithms for the the study of complex materials, properties and processes in realistic condition, far beyond the current realms.
- At the same time, MaX is working to radically enhance the performance of the flagship codes in terms of scaling, robustness, and usability, and will make them ready for the forthcoming exascale hardware architectures.

In this way, MaX is designing and implementing a sustainable approach of relevance beyond its core codes and domain.

QUANTUM ESPRESSO (Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization) is an integrated suite of packages, implementing density-functional theory (DFT) for atomistic simulations based on the electronic structure, as based on a **pseudo-potential plane-wave** implementation. It is released under the GNU GPL licence, and includes the most advanced levels of the theory.

Number of forum/mailling-list subscribers	2.000
New releases since 01/09/2015	5.2.1 (24/09/2015)
	5.3.0 (09/01/2016)
	5.4.0 (27/04/2016)
Unique downloads since 01/09/2015	5.2.1: 3.750
	5.3.0: 1.000

Main development steps planned:
 Implementation of AiiDA plugins. [done]
 Implementation of new scientific features. [done and planned]
 New Data Interfaces and parallel I/O support. [done and planned]
 MPI optimization & OpenMP layers. [planned]
 Python post processing application suite. [planned] - Major Code Refactoring. [planned]

SIESTA is a density-functional code able to perform efficient electronic structure calculations and ab-initio molecular dynamics simulations of molecules and solids. SIESTA efficiency stems from the use of strictly **localized basis sets** and from the implementation of **linear-scaling algorithms** which can be applied to suitable systems. A very important feature of the code is that its accuracy and cost can be tuned in a wide range, from quite exploratory calculations to highly accurate simulations.

Number of forum/mailling-list subscribers	1.200
New releases since 01/09/2015	4.0 (beta)
Unique downloads since 01/09/2015	2.000

Main development steps planned:
 Change in policy licensing (Open Source) [done] - Implementation of AiiDA plugins [done]
 Implementation of new scientific features [done and planned]
 New Data Interfaces and parallel I/O support [started]
 MPI optimization & OpenMP layers [planned] - Major Code Refactoring [planned]





YAMBO is a code that implements ground-state as well as excited-state properties in an ab initio context using **plane waves and pseudopotentials**. YAMBO is released within the GPL license and is currently interfaced with *QUANTUM ESPRESSO* and *Abinit*. The code implements MBPT and advanced orbital dependent functionals within DFT in order to allow the user to calculate a wealth of physical properties: reliable bandgaps, band alignments, defect quasiparticle energies, optical and out-of-equilibrium properties.

Number of forum/mailling-list subscribers	600
New releases since 01/09/2015	4.0.2 (devel) (15/10/2015) 3.4.2 (stable) (15/02/2016)
Unique downloads since 01/09/2015	4.0.2: 340 3.4.2: 170

Main development steps planned:
 Implementation of AiiDA plugins. [done]
 Setup of a benchmark suite. [done]
 Implementation of new scientific features. [done and planned]
 Parallel Linear Algebra Implementation. [started]
 MPI optimization & OpenMP layers. [started]
 Kernel modularization. [planned]
 Major Code Refactoring. [planned]

FLEUR (Full-potential Linearized augmented plane wave in EUROpe) is a code family for calculating ground-state as well as excited-state properties of solids within the context of density functional theory treating all electrons on the same footing. It is based on the full-potential linearized augmented plane wave method. The FLEUR family consists of three codes: (i) a versatile DFT code for the ground-state properties; (ii) A Green-function implementation used to calculate ballistic transport properties through planar junctions, and (iii) the SPEX code, an implementation of many-body perturbation theory (MBPT) for the calculation of the electronic excitation properties of solids.

Number of forum/mailling-list subscribers	2500
New releases since 01/09/2015	Fleur MaX-Release-1 31/05/2016 (planned)
Unique downloads since 01/09/2015	250

Main development steps planned:
 Implementation of AiiDA plugins [started]
 New Data Interfaces and parallel I/O support [started]
 Implementation of new scientific features [planned]
 MPI optimization & OpenMP layers [planned]
 Major Code Refactoring. [planned]



SIESTA IS NOW RELEASED UNDER GPL OPEN SOURCE LICENCE

Following the agreement of moving the code under a new fully Open Source compliant license (GA, IPR section), the SIESTA developers took the action to change the licensing conditions for the code. Starting in the Spring of 2016, SIESTA will be released under the GPL open-source license (https://en.wikipedia.org/wiki/GNU_General_Public_License). In the past SIESTA had always been free for academic use, but re-distribution was not permitted. It is expected that the move to an open-source license will result in a more flexible and dynamic development for the program. On the one hand, SIESTA will be able to incorporate functionalities already existing in other GPL codes. On the other, the barrier for contributors will be lowered, as new developments will be more easily re-distributed. With this change, all the flagship codes in the MaX consortium are open-source.

MATERIALS INFORMATICS ECOSYSTEM: WORKFLOWS AND DATA

WP1-WP2-**WP3**-WP4-WP5-WP6-WP7

MaX offers a materials informatics ecosystem for automated high-throughput calculations and the automatic storage of data in graph databases: a working environment that enables workflows and turnkey solutions, as well as sharing of data and workflows, and guarantees provenance, storage and preservation, reproducibility, reuse, as well as data analytics.

This effort is performed in close collaboration with **Marvel**, a long-term Swiss effort coordinated by EPFL, and largely based on one of our flagship codes, i.e., **AiiDA**.

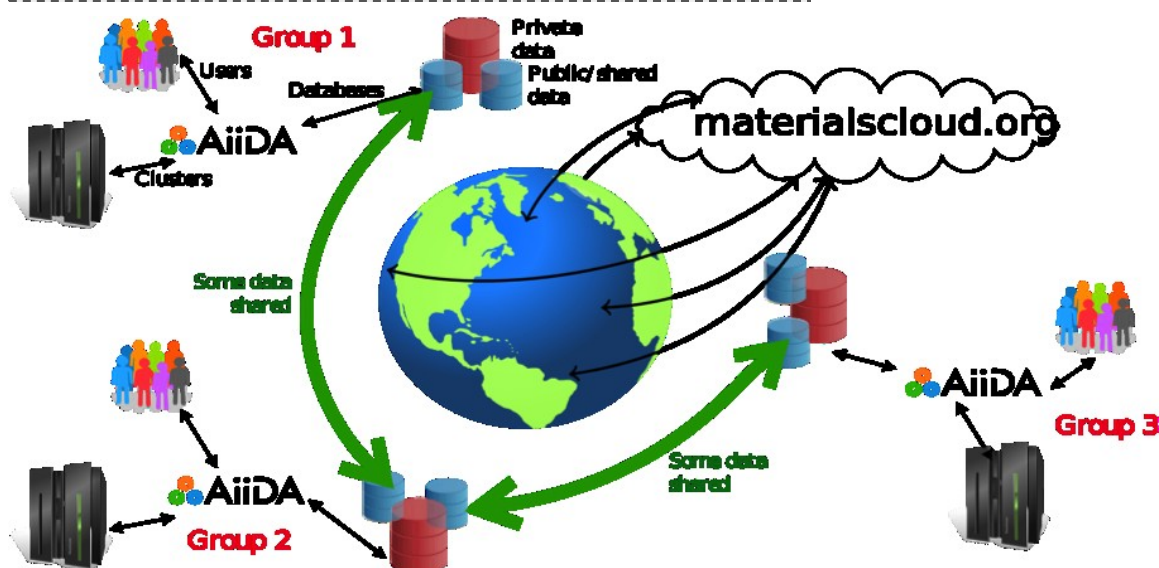
At the same time, code interoperability and scalable programming is addressed by PALENQUE (see below).



AiiDA (Automated Interactive Infrastructure and Database for Atomistic simulations) is a Python materials' informatics framework to manage, store, share, and disseminate the workload of high-throughput computational efforts, while providing an ecosystem for materials simulations where codes are automatically optimized on the relevant hardware platforms, and complex scientific workflows involving different codes and datasets can be seamlessly implemented and shared.

AiiDA is designed around the four pillars of materials' informatics: Automation, Data, Environment, and Sharing. At the low-level, AiiDA takes care of automation and data storage for the management and safeguarding of calculations, data and workflows. At the user-level, it provides an advanced and intuitive research environment for accelerating scientific discoveries, and sharing capabilities to enable collaborative research. A cartoon of the materials informatics ecosystem enabled by AiiDA is shown below.

PALENQUE (Python Abstraction Layer for Quantum Engines) is a Python framework aimed at: i) reducing code duplication by moving common features that require little communication and computational burden outside of the Quantum Engines (QEs); ii) facilitating the implementation of new algorithms that are shared by multiple QEs. This is obtained by delegating to an external wrapper written in a high-level language the evaluation of increasingly complex functions.





EXASCALE CHALLENGE

WP1-WP2-WP3-**WP4**-WP5-WP6-WP7

MaX addresses the challenges of porting, scaling, and optimizing materials science application codes for the exascale platforms in order to deliver best code performance and improve users productivity on the upcoming architectures. This activity is fundamental for the sustainability of the MaX ecosystem, which is crucially based on the excellence of codes, which, in turn, requires their maintenance at the technological frontier.

Sustained performance, energy awareness, code fault tolerance, task concurrency and load balancing, numerical noise and stability, are some of the exascale related challenges addressed by MaX WP4.

The overall objective of the exascale challenge is to consolidate and develop the competences and the services enabling materials science to exploit next generation systems towards the exascale. The main tasks of MaX WP4 include advanced programming paradigms, novel algorithms, domain specific libraries, in-memory data management, and software/hardware co-design:

advanced programming models are considered and possibly implemented to deal with the architectural paradigm change imposed by the exascale roadmap. For instance, parallelism strategies beyond hybrid MPI+openmp need to be assessed and possibly exploited. Dedicated profiling of the flagship codes is required in this respect.

novel algorithms are considered (or devised), evaluated, and implemented in order to best cope with the massive parallelism imposed by the hardware evolution towards exascale. Algorithms suited for large parallel performance are expected to play a major role.

the use of **domain specific libraries** (as opposed to general purpose libraries) is pursued as much as possible within the flagship codes. This will permit to exploit domain specific knowledge to improve on the library performance as well as to hide at the very low level HW-architectural complexity. On the one hand this will allow for easier exploitation of specific HW (e.g., accelerators), while on the other hand, it will also make libraries with advanced and optimized algorithms available to the wider materials science community.

HW-SW co-design is one of the central activities of WP4, supported by the action of two dedicated partners (E4, KTH) together with CINECA. A tight connection and data exchange with HW manufacturers is foreseen as beneficial to both sides: materials science community codes can provide relevant user feedback to manufacturers, while also indicating needs and eventually steering technology customization. Networking with manufacturers has started and is undergoing (see success story below).

The flagship codes are being profiled and continuously benchmarked for the whole duration of MaX, to allow full tests of any new solutions (WP1-WP4 collaboration).



CO-DESIGN: GETTING STARTED AND BUILDING THE NETWORK

Within the scope of the co-design activities of WP4, MaX started discussing with several players (INTEL, IBM, ARM, etc.) involved in developing technologies along the exascale roadmap. Discussions started at SC15, and continued in the first months of 2016, pointing out that HW manufacturers prefer to work on co-design using less complex software with respect to full featured applications (the latter are difficult to manage and their performance and profiling is often too dependent on the input dataset). In reply to that, MaX partner CINECA has developed two mini-app's concerning domain specific FFT and linear algebra (not originally included in the DOW, but adding effort on top of what was already committed), easy to be ported to new hardware, eliminating all the complexity of the full application but being accurate in reproducing numerical functionalities. The mini-app work was presented at the Computing on Low-power Architectures (COLA) workshop (February 2016, Ferrara). Based on the mini-app initiative, a successful collaboration started with the Mont-Blanc project. MaX representatives (CINECA) proposed the possibility to use the newly developed mini-app's to contribute to the application co-design and validation of the Mont-Blanc exascale architecture within the Mont-Blanc project. The discussion with Mont-Blanc PIs started at the COLA workshop and continued a few weeks later in a dedicated meeting with the Mont-Blanc team working on application porting and benchmarking. Mont-Blanc is now using the MaX mini-apps the results were presented at the 2016 Exascale Applications & Software Conference (EASC 2016) in April in Stockholm.

At the same time, co-design initiatives are promoted by MaX within several partnerships. For example:

- a FET-PROACTIVE proposal was submitted by CINECA together with IBM on variable precision arithmetics (co-design on materials science applications planned);
- a formal contract is foreseen to be signed by CINECA and INTEL on co-design themes;
- Quantum-ESPRESSO was selected for the benchmark suite of the PRACE (Pre Commercial Procurement): it is thus used to design, test, and validate the involved prototype systems (about 1 1PFlop each) targeting a European architecture with top energy efficiency.

SERVICE CATALOGUE

WP1-WP2-WP3-WP4-WP5-WP6-WP7

MaX is a user-driven CoE, built from and aimed at operating within the wider computational materials science community. MaX

- provides a number of services to end-users (from academia and industry) interested in materials science simulations;
- facilitates the creation of a community of users built around the flagship codes;
- sets up relevant actions to facilitate the connection with possible users/customers.

A number of services was devised and developed, in particular following known business models appropriate for open source software. In a first phase, services are operational in a beta version (May 2016).

We expect that this first phase will allow for a realistic estimate of the possible relevance of services for the long-term sustainability of MaX (pay-for services). A rough count of the impact of services, obtained during a prototypal, pre-launching phase, are reported in the 'MaX in numbers' page.

Here follows the service catalogue currently put in place by MaX. The services will be accessible through MaX users' portal.

MAX CODE DOWNLOADING SERVICE

New high-quality releases of its open-source flagship codes are a key output of MaX. The Center offers to all users:

- Downloading of last releases and documentation
- Access to a repository of benchmarks [planned].

MAX BASIC SUPPORT

MaX ensures basic support for free to all users of its codes:

- Forum/mailling- list support for codes related issues;
- Forum support for materials science and HPC issues [planned];
- Knowledge base navigation [planned].

MAX HELP-DESK

Direct contact help-desk service for:

- Code utilization (focus on performances and HPC optimization);
- Input preparation and output analysis;
- Code personalization (small modifications).

MAX ADVANCED SUPPORT

Direct contact help-desk service dedicated to HPC users (specifically for proposal submission):

- Specific technical issues (scaling, CPU and memory requirements);
- Guided choice of appropriate codes for specific research context.



MAX ADVANCED CONSULTING

Dedicated on site advanced consulting focused on industrial needs:

- Scientific case, workflow definition;
- Dedicated code development;
- Code porting;
- Full support to complex research issues.



MAX DEDICATED TRAINING

Education and training initiatives

- Schools and Courses organization;
- Specific modules;
- Training through research in the MaX Labs;
- Dedicated courses and tailored programs.



MAX FORGE ENVIRONMENT (PLANNED)

Access to a 'MaX integrated development environment (IDE)' open to developers of scientific software in the field.



QUANTUM ESPRESSO goes to market

Doing business with open-source software is a considerable challenge. The Quantum ESPRESSO developers' group has taken up the challenge by signing an important commercial agreement with a leading scientific software company, Schrödinger LLC (<http://www.schrodinger.com>), under the umbrella of the Quantum ESPRESSO Foundation (<http://foundation.quantum-espresso.org>), which coordinates the efforts of several MaX members (SISSA, CINECA, EPFL, ICTP, among others) also leveraging the consultancy expertise of another MaX member (CloudWeavers). Following this agreement, Quantum ESPRESSO will be included in the molecular and materials modeling suite commercialized by Schrödinger LLC, bundled with proprietary software. The coexistence in a same product of open-source and proprietary software components is requiring a considerable technical effort, which we believe will be of great benefit for the entire community of (non-commercial) users of the Quantum ESPRESSO suite of codes, and will constitute an example of original business model of great interest for the open-source scientific-software community at large. Within the MaX project, CloudWeavers helped the group since the initial phases of negotiation, by drafting a proposal, consulting on legal matters and licensing, by providing effort and cost estimates, and giving advice on the content and finalization of the commercial agreement. The contract between Schrödinger and the Quantum Espresso Foundation was signed in spring 2016.

TRAINING AND EDUCATION

WP1-WP2-WP3-WP4-WP5-**WP6**-WP7

MaX contributes to the community effort to bridge the skill gaps – both present and future— that may hinder the full deployment of Europe’s potential in HPC & Material Science.

The existing training and education offer in Europe is rather rich, but would greatly benefit of a stronger integration between the HPC and the materials domain components at all levels. MaX focuses on integrating and complementing the existing offer through specific activities. Our offer includes workshops and schools on HPC applications in computational materials science, university modules and materials at both undergraduate and graduate level, and the possibility of training through research in MaX laboratories. Diversity and gender balance are constant objectives of MaX initiatives.

Teaching material and Open Online courses will be available in the dedicated section of the User Portal. Forthcoming schools and workshops on HPC applications in computational material sciences can be found in the events section and in the dedicated section of the User Portal. Specific training activities for industrial end-users are offered as a dedicated service.

MAIN ACTIONS & EVENTS

A list of selected events offered and planned by MaX follows:

1. Specific Training Workshops/Courses

- √ Tutorial on AiiDA, November 2015.
- √ Linear Response workshop 2016, January 2016.
- √ Joint MCC-UKCP-EPC Workshop on Ab initio Periodic Codes, January 2016.
- √ Python for computational science, January 2016.
- Course on HPC Numerical Libraries, Winter 2016.
- MARVEL/MaX/Psi-k Tutorial about AiiDA platform, June 2016.
- Hands-on schools for each flagship code, 2016/2017.
- PRACE/MaX PATC, 2017.

2. University course modules

- √ Master in High Performance Computing, February and July 2016.
- Course on computational Physics at University of Modena and Reggio Emilia, 2016.
- Master Course at the German Research School for Simulation Sciences, 2017.

3. Massive Open Online Courses

Preparation of video lectures during workshops and schools to be distributed through the MaX communication channels.

PILOT USER CASES

WP1-WP2-WP3-WP4-WP5-WP6-WP7

MaX is currently working on four 'Pilot Cases' which face open problems that MaX contributes to solve in close contact with leading industrial partners. The Pilot Cases are meant as a test ground for MaX working approach, which will then be applied to similarly challenging problems that will emerge from MaX users and community.

Importantly, the developed packages and workflows will constitute the basis for a MaX 'market-place' where solutions developed for a given problem will be made available and tailored to other end-users. This opportunity is expected to enable a rapid response to shorter-term issues, and could be typically well suited, e.g., for SMEs.

The four pilot cases are:

- Pilot Case 1. Computational protocol for friction and tribochemistry.
- Pilot Case 2. Computational protocol for understanding thermal energy storage in molten salts and nanofluids.
- Pilot Case 3. Computational protocol for simulating the colour optical properties of natural dyes for food industry.
- Pilot Case 4. Design and discovery of optimal solid-state electrolytes in research and innovation, both in industry and academia, who explore materials discovery and rely on computer experiments.

COMPUTATIONAL PROTOCOL FOR FRICTION AND TRIBOCHEMISTRY

(Key team: M.C. Righi, CNR)

INDUSTRIAL PARTNER: **Total SAS and Toyota Europe**

INDUSTRIAL INTEREST: Understanding and control of friction are key topics in manufacturing and in any application with parts in relative motion, with huge implications, e.g., in the automotive sector. Stress-assisted chemical reactions, occurring between two surfaces in relative motion, play a central role in tribological phenomena such as wear, which is ruled by bond breaking/forming across the interface, and boundary lubrication, where interfacial molecules react with the contacting surfaces and modify their properties of adhesion and resistance to sliding. This is the basic principle for the functionality of lubricant additives, e.g. in motor oils, and it also explains the influence of air humidity on the frictional properties of solid lubricants, such as diamond/diamond like carbon (DLC).

TARGET: Developing a computational protocol to model tribochemistry processes occurring in solid and boundary lubrication, based on a combination of advanced ab-initio simulations and a parameterization of the ab-initio potential energy landscape to extend time/length scales.

PILOT CASE 1

Computational protocol for understanding thermal energy storage in molten salts and nanofluids

(Key team: P. Ordejon, ICN2)

INDUSTRIAL PARTNER: **Abengoa Research**

INDUSTRIAL INTEREST: Innovation is a key factor for realising the potential of novel, renewable and clean energy sources to compete with fossil fuels. Improving the efficiencies and thus lowering the cost of energy generation is essential for the economic viability of novel, renewable and clean energy sources. Solar thermal energy is one of the most competitive alternatives: the heat generated can be stored in a heat storage medium by means of an intermediate heat transfer fluid, for further transportation and use.

Molten salts are one of the preferred options used by industry. Optimising the thermal storage and transport properties of molten salts is therefore key for the global efficiency of these technologies. One of the options for improving these properties, in particular thermal conductivity and specific heat, is to introduce nanoparticles dispersed in the molten salt. Simulation plays a very important role in this research and innovation process, as producing reliable experimental data for these systems is difficult and expensive. Within MaX, we will collaborate with Abengoa Research to elaborate computational protocols for the determination of the key thermal parameters of molten salts containing nanoparticles. The protocols will then be made public, and will be tested and used by Abengoa Research, within their proprietary activities.

TARGET: Elaborating computational protocols for the determination of the key thermal parameters of thermal storage fluids like molten salts, and to predict and explain the modification of these properties by the addition of nanoparticles (the so-called nanofluids).

Computational protocol for simulating the colour optical properties of natural dyes for food industry

(Key team: S. Baroni, SISSA)

INDUSTRIAL PARTNER: **Mars Chocolate**

INDUSTRIAL INTEREST: In order to comply with EU regulations on food safety, many colorants commonly employed in the food industry will be substituted with natural ones. However, the colour palette from natural sources is still incomplete, and the understanding of the relation between the chemical structure and the optical properties of natural pigments inadequate, thus making the chase of molecules with custom-designated chromatic properties a blind search.

TARGET: Designing and implementing a simulation protocol to assist industrial research in the identification of the most suitable natural dyes to express custom-designated hues of colours (particularly in the purple-blue gamut), and to apply it to the screening of anthocyanins.

Design and discovery of optimal solid-state electrolytes

(Key team: N. Marzari, EPFL)

INDUSTRIAL PARTNER: **Bosch Research**

INDUSTRIAL INTEREST: Improving performance and safety of electrochemical storage systems to reduce amount of greenhouse gas emitted by vehicles.

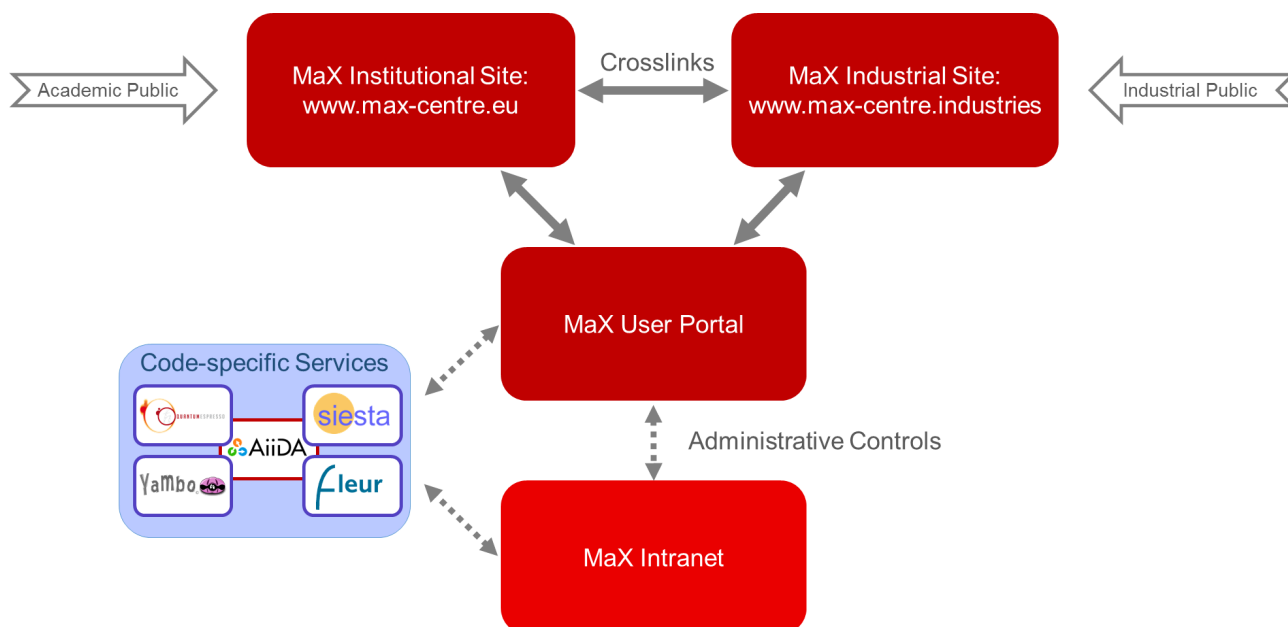
TARGET: Search for new materials for solid-state electrolytes for lithium ions and protons in a high-throughput screening approach, by understanding diffusion processes and finding accurate descriptors for ionic conductivity.

WEB SERVICE, INTRANET AND USER PORTAL

The user base of MaX is at least twofold in nature, comprising on one side experts in frontier computational developments in academia or industry, and on the other side end-users possibly working in a SME environment. The latter are sometimes less familiar to cutting edge technological developments of materials applications, and are probably best approached by emphasizing the possible impact of materials simulations in different fields of industrial interest.

In order to efficiently reach both targets, web access to MaX is guaranteed by two interconnected websites, resting on www.max-centre.eu and www.max-centre.industries IT-domains: each is designed for a specific segment of MaX user base. These two sites are crosslinked, and service provisioning is ensured through a common User Portal.

The access-restricted Intranet Portal and the intranet communication suite complete the MaX IT-infrastructure. The **User Portal** manages the (possibly restricted) user access to code-specific services (see the service section for a description of the delivered services). The **Intranet Portal** provides services to the MaX internal community (about 70 users, at the time of writing). It has been designed to ensure a collaborative platform, facilitating circulation of ideas among MaX partners, and a knowledge repository. It is based on the Google apps cloud technology, with specific personalization.



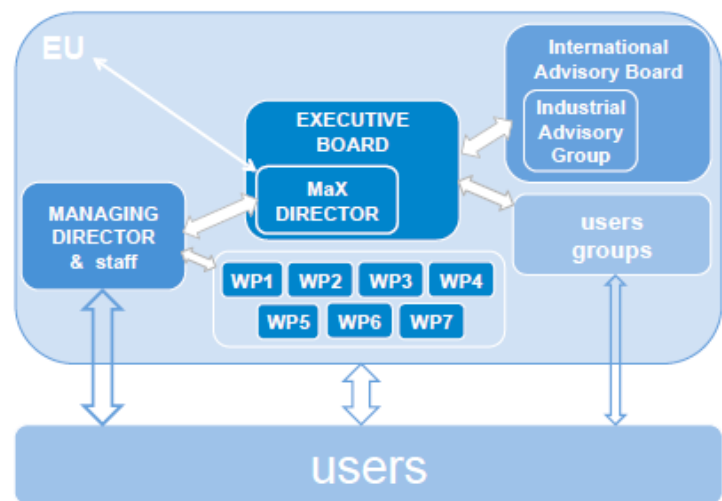
ORGANIZATION & GOVERNANCE

MaX is guided by an **Executive Board (EB)** and by the **Director**. They coordinate the actions of the WPs towards common objectives, monitor the development of the activities and the interactions with users, analyse any difficulties/new opportunities in the CoE development, and determine the necessary actions. The **Executive Board** includes the PIs of all nodes. Thus it also includes WP1-WP6 leaders; the leader of WP7 is an invited participant.

The **WP leaders** coordinate the activities of their WPs, make sure that these proceed smoothly, and report the main achievements to the Director and the EB.

The **International Advisory Board (IAB)** advises the Director and the EB on the main strategic choices that may be needed during MaX, on evaluation of the overall progress. It will also help to shape the evolution of MaX after the end of the project.

The MaX **management team** (Executive manager and staff) ensures the implementation of the goals defined by the EB and Director, manages service access and offers a single and easy entry point to the users.



Executive Board members

Elisa Molinari, CNR NANO
Stefano Baroni, SISSA
Pablo Ordejón, ICN2
Stefan Blügel, FZ-Jülich
Nicola Marzari, EPFL
Carlo Cavazzoni, CINECA
José Maria Cela, BSC
Thomas Schulthess, ETH Zurich
Erwin Laure, KTH
Piero Altoè, E4
Carlo Daffara, CloudWeavers Ltd
Ivan Girotto, UNESCO-ICTP

WP Leaders

WP1 Stefano Baroni, SISSA
WP2 Pablo Ordejón, ICN2
WP3 Nicola Marzari, EPFL
WP4 Carlo Cavazzoni, CINECA
WP5 Carlo Daffara, CloudWeavers Ltd
WP6 Stefan Blügel, FZ-Jülich
WP7 Andrea Ferretti, CNR NANO

International Advisory Board Members

Alessandro Curioni, IBM Research Zurich & IBM Europe
Giulia Galli, University of Chicago and MICCoM
Kersti Hermansson, Uppsala University and European Materials Modeling Council (EMMC)
Boris Kozinsky, Bosch R&T Center Boston
Jens Norskov*, Stanford University
Marie-Christine Sawley, Intel Paris Exascale Laboratory
Erich Wimmer, Materials Design and EMMC
TBC, Graphene Flagship

NETWORKING, COMMUNICATION, DISSEMINATION

WP1-WP2-WP3-WP4-WP5-WP6-**WP7**

A first list of interactions/collaborations launched by MaX **within the broader European ecosystem** of Materials and HPC research:

- . Psi-k community: a 'strategy' meeting, with the participation of the materials-related CoEs, was held in San Sebastian to plan joint activities (September 2015); a joint 'Psi-k highlight' paper is being prepared together with ECAM and NOMAD CoEs, and should appear in May 2016.
- . NFFA-Europe (Nanoscience Foundries and Fine Analysis: www.nffa.eu). A EU (H2020-INFRAIA) network that provides "Transnational Access" to users, to research infrastructure in nanoscience, including Theory and Simulation. We aim at including the MaX services for simulation software development and workflows and protocols for specific needs, through the access forms for the application of services offered by NFFA.
- . EMMC (European Materials Modeling Council). We have joined the EMMC and its activities, aiming at becoming a relevant actor in its definition of the EMMC Roadmap for 2018-2020. MaX has included two members of the EMMC in its International Advisory Board.
- . Graphene Flagship (GF). Conversations are ongoing to establish a formal collaboration between MaX and the GF, so that the GF research and industrial teams gain direct access to the services provided by MaX. A meeting with the Directorate and Strategic Board of the Flagship was held in Genova, April 2016.
- . MARVEL: this long-term project supported by the Swiss NSF is a key partner of MaX on most activities involved in WP3 and data.
- . ETP4HPC: MaX contributed to the survey and discussion promoted by the EXDCI support project, and to the ETP4HPC work-group on software engineering. We are also extremely interested in the EsD (Extreme scale Demonstrator) discussion.
- . PRACE: MaX is collaborating with PRACE on several training activities, and directly supports the Materials Research community towards high quality submissions to PRACE.
- . IPCEI-HPC-BDA: coordination with leading stakeholders from Italy, France, Luxemburg, and Spain, in view of an "Important Project of Common European Interest" (IPCEI) on High Performance Computing and Big Data enabled Applications (HPC-BDA). MaX will contribute especially to the Technology and the Large Scale Application pillars. A preliminary submission is planned for May 2016.
- . SESAMEnet and EDISON: a first attempt to coordinate in view of joint training activities and proposals.
- . 'From volume to value': coordination action of the Emilia Romagna Region on Big Data and HPC applications. MaX coordinates activities for the Materials domain. A publication appeared in February 2016.

A first list of selected interactions/collaborations launched at **international level**:

- . A coordination forum, promoted by G. Galli (Chicago), among the three newly established computational materials science centers in the US and the three established in Europe, one in Switzerland and at least one in Japan. The senior PIs of these centers, together with some of the PIs of other major materials effort, will convene and discuss their respective strategic views, ways to collaborate and ways to benefit from each other, e.g., by developing complementary capabilities. A

meeting is planned in Paris in Spring 2017.

- . Intense collaborations with ORNL and the DoE lead Exascale Computing Project, as well as Tokyo Institute of Technology, on library development at the linear algebra level. Further collaborations with BNL and ORNL at the level of QE.
- . Collaborations with UC Berkeley and LBL lab (Profs. Lin Lin and Chao Yang), on the development of efficient algorithms for massively parallel architectures. In particular, the implementation of the PEXSI method in SIESTA.
- . Collaboration with UNESP, Sao Paulo, Brazil (Prof. A. Rocha and Dr. G. Feliciano) on protocols for the calculation of quantum electronic transport in molecular devices in the presence of liquid environments. (The protocols comprise classical Molecular Dynamics simulations of the molecular bridge immersed in the liquid, the QM/MM partition of the system to compute the electronic properties at selected snapshots of the MD runs, and Non-Equilibrium Greens Functions calculations of the electronic transport in the presence of the potential created by the MM partition to compute the electrical characteristics of the device.)
- . MaX is especially active in developing countries, thanks to its collaboration with the ICTP partner. Through the ICTP network/support, most of MaX training and education activities are promoted and made available to researchers from such countries. Examples include MaX modules within the Trieste Master in HPC, and the Quantum Espresso School planned for January 2017.

Selected Communication/Dissemination contributions:

- . 2015 Sep 7-10: Psik conference, San Sebastian, Spain, **Elisa Molinari**, plenary presentation "MaX: Materials design at the Exascale".
- . 2015 Sep 28 - Oct 2: Intel Xeon Phi User Group (IXPUG) Annual Meeting 2015, LBNL Berkeley, CA, **Andrea Ferretti and Fabio Affinito**, Invited Talk "Yambo and Quantum ESPRESSO as test cases for code optimization towards exascale".
- . 2016 Mar 14-18: APS March Meeting, Baltimore Maryland, **Andrea Marini**, Invited Talk "The Yambo code: a comprehensive tool to perform ab-initio simulations of equilibrium and out-of-equilibrium properties".
- . 2016 Apr 25-29: Exascale Applications & Software Conference (EASC) 2016, **Carlo Cavazzoni** "Software and services for materials design at the exascale: the challenge, the mission, the vision".

Selected Publications:

- . K. Lejaghere et al, "Reproducibility in density functional calculations of solids", Science 351, 1415 (2016).
- . N. Marzari, "Materials modelling: the frontiers and the challenges", Nature Materials 15, 381 (2016).
- . A. Marcolongo, P. Umari, S. Baroni, "Microscopic theory and quantum simulation of atomic heat transport", Nature Physics 12, 80-84 (2016).
- . G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, B. Kozinsky, "AiiDA: automated interactive infrastructure and database for computational science", Comp. Mat. Sci. 111, 218 (2016).
- . L. Barney, "Supercomputers aid in quantum materials research", Scientific Computing (2016), <http://www.scientificcomputing.com/articles/2016/04/supercomputers-aid-quantum-materials-research>.

In the following two Annexes are given:

ANNEX I – WP Actities

ANNEX II– Pilot Cases

They provide raw data as collected during MaX life
for internal communication and reporting.

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