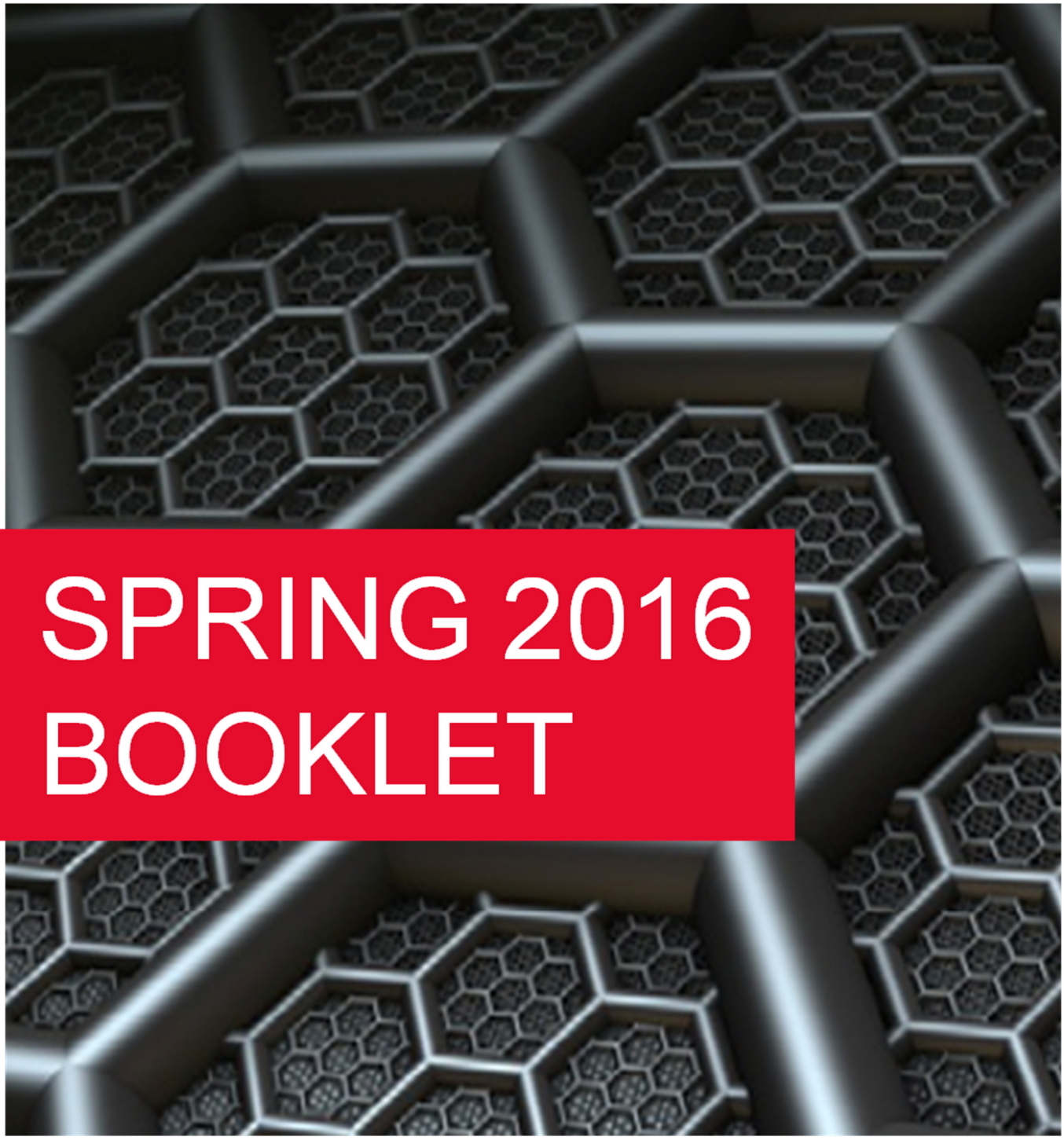

SPRING 2016 BOOKLET

MaX

Materials Design at the Exascale

European Center of Excellence in materials modelling, simulations and design

ANNEX I — WP Activities

WP1

The software development plan was defined in D1.1, which addresses the organisation of new features into three groups to be implemented in three major relaese (R1-R3). D1.1 was delivered to the European Commision on March 1, 2016

QUANTUM ESPRESSO

Number of Software releases: 3

- QUANTUM ESPRESSO 5.2.1 24 September 2015
- QUANTUM ESPRESSO 5.3.0 9 January 2016
- QUANTUM ESPRESSO 5.4.0 27 April 2016

Number of planned new features implemented. 2

- Implementation of the new schema-compliant XML I/O for pw.x
- Experimental version of the ThermoPW code for the computation of thermal

material properties using QUANTUM ESPRESSO quantum engines. For the features recently implemented see the the WP1 Tasks advancements list.

Number of unique downloads of the code. (total number of accesses to the download link (includes failed, repeated accesses and bots);

- QUANTUM ESPRESSO 5.2.1 > 75000
- QUANTUM ESPRESSO 5.3.0 > 20000

Number of journal citations since Sept. 2015: > 600

Number of forum/mailing-list subscribers: > 2000

SIESTA

Number of Software Releases: 1

- Siesta 4.0-β

Number of planned new features implemented 2

Spin-Orbit-Coupling capability;

implementation of PEXSI non diagonalizing solver.

Number of unique downloads of the code. > 2000. (10% of access requests to the download site)

Number of journal citations since September 2015: > 600.

Number of forum/mailing-list subscribers: > 1200.

YAMBO

Number of Software Releases: 4

- YAMBO 4.0.2 (devel) October 2015
- YAMBO 3.4.2 (stable) 15 Febbruary 2016
- YAMBO 4.0.3 (devel) May 2016
- YAMBO 4.1.0 (devel) planned for July 2016 (MaX Release 1)

Number of planned new features implemented : 2

- Implementation of the terminator technique to accelerate the convergence on the sum over empty states when computing the GW self-energy within the plasmon pole model.
- Development of the yambo-py scripting tools as, task-oriented parallelization strategy based on scripting tools. (http://www.yambo-code.org/doc/yambopy.php)

Number of unique downloads of the code:

- YAMBO 4.0.2 : 669
- YAMBO 3.4.2 : 344

Number of Journal Citations since September 2015: 40

Number of forum/mailing-list subscribers:

- Number of svn (registered) users: 186
- Number of yambo forum users (registered): 491
- Number of active developers: 14

FLEUR

Number of Software Releases: 1

Fleur MaX-Release-1 α: to be released in May 2016

Number of planned new features available 0

Number of unique downloads of the code 2565 (number of registered accounts authorized for downloads. Few of them are actually used. The estimate of unique downloads will be improved in the future

Number of journal citations:

- 2015: 410
- 2016: 11

Number of forum/mailing-list subscribers 2565 (coincident with the number of registered accounts above.

Short description of software releases

QUANTUM ESPRESSO

QUANTUM ESPRESSO 5.2.1 released 24 September 2015

- svdW-DF: a proper spin version of van der Waals (PRL 115, 136402 (2015);
- XSpectra: various improvements and extension;
- ESM: various improvements, constant bias calculations(PRL 109, 266101 (2012) for both pw.x and neb.x;
- standard F2003 calls to: get_environment_variable, get_command_argument, command_argument_count, flush, are used everywhere instead of wrappers;

QUANTUM ESPRESSO 5.3.0 released 9 January 2016

- FFTXlib: FFT handling subroutines re-factored in a self-contained library;
- projwfc.x: projected density of states (PDOS) with PAW projectors and allelectron basis functions;
- X3LYP,B3LYP and B3LYP hybrid functionals;
- New coding of the Fermi Surface Plotting Tool
- Linear algebra parallelization made independent of its parent communicator

QUANTUM ESPRESSO 5.4.0 to be released 27 April 2016

- LAXlib library, containing routines for parallel subspace diagonalization
- Calculation of Magnetic anisotropy energy in the limit of small spin-orbit coupling using the Force theorem

Support for FFT with ARM Performance LibraryNon-blocking FFT communications

- Solution of Bethe-Salpeter equation added to GWL
- Support for QM-MM using MPI
- Phonons with vdw-DF and with DFT-D2
- I/O reduction: k+G indices "igk" no longer written to and read from file, files not opened unless explicitly required or needed;
- more band parallelization, improvements to EXX parallelization;
- First step towards modularization of Linear-Response codes: common module moved to new directory LR_Modules.

SIESTA

Siesta 4.0 Beta

- advancements in the implementation of the spin-orbit-coupling capability;
- implementation of spin-polarization capability the SIESTA-PEXSI iterative solver;
- implementation of the N-electrode method in Trans-Siesta.

Progresses in WP1 Tasks

QUANTUM ESPRESSO

• Code Profiling. Collection and definition of significant benchmarks.T1.1.1
• Incremental improvements of parallel performances. More parallelization over bands. Reduction of the communication overhead in FFTs T1.1.1
• Modularization: replacement of code-specific functions with domain-specific libraries and extensive code reorganization with collection.T1.1.1 and T1.1.2
• Reduction of I/O T1.1.2
• Experimental version of XML input output for pw.x completed. T1.1.3
• XML IO for all the QUANTUM ESPRESSO suite in progress T1.1.3;
• Testing of HDF5 based new bynary output for massive bynary data sets T1.1.3
• Many progresses in the implementation of the ThermoPW codes for computing material properties T1.2.2:
– added the possibility to fit the energy with a fourth order polynomial;
– improved the recover abilities of the code;
– support for the calculation of the X-ray diffraction spectra;
– started to implement finite pressure calculations;
– thermal expansion from Gruneisen parameters for hexagonal, tetragonal, and orthorombic solids (experimental);
– Introduced support for the Debye model

SIESTA

• Setup of benchmarking and profiling framework for SIESTA to be used during the project for performance assessment (In collaboration with BSC and WP4)T1.1.1;
• encapsulation of data structures in reference-counted objects to simplify memory handling T1.1.2 ;
• installation of a reference AiiDA instance at BSC to test the forthcoming SIESTA plugin; T1.1.3
• Preliminary implementation of parallel-I/O features using netcdf-4, which has hdf5 as the storage layer. T1.1.3
• Design and implementation of new development and release workflows to accomodate the change in licensing policy for SIESTA. There is already a website http://launchpad.net/siesta to host the code and related development material.

YAMBO

• Implementation of the terminator technique (X. Gonze, F. Bruneval, PRB 2012) to accelerate the convergence on the sum over empty states when computing the GW self-energy within the plasmon pole model.T1.2.4
• Setup of a test, benchmark, and profiling suite to be used during the project for performance assessment T1.1.1;
• Parallel performance and profiling sessions. In collaboration with WP4 (CINECA) we started profiling and benchmarking yambo (one profiling session; one benchmark data collected) T1.1.1
• Improvement and stabilization of different strategies of MPI parallelization, for extended systems (k-dispersed) and isolated systems (number of states). The present devel (4.0.2) is foreseen to become the stable yambo release on August 2016 with release (4.1.0) [done/to be finalized] T1.1.1;
• New openmp parallelization of the RPA linear response calculation (targeting efficiency over a large number of openmp threads). T1.1.1 [done]
• Development of the yambo-py scripting tools as, task-oriented parallelization strategy based on scripting tools; T1.1.1 (http://www.yambo-code.org/doc/yambopy.php);
• Parallel linear algebra [ongoing] T1.1.1;
• Implementation of the AiiDA plugin for yambo (together with Gianluca Prandini and Henrique Miranda) [ongoing] T1.1.3 .

FLEUR

• Performance improvement T1.1.1
– definition of the set of benchmarking tests ;
– benchmarkig of the code with special focus on the matrix generation;
– Replacement of Fortran I/O for eigenvectors with memory storage using one sided MPI communication or alternatively disk-storage using HDF5-IO;
• Modularization: starte the code refactoring to include Fortran data-types T1.1.2
• Implementation of new features for Communication and Interoperability T1.1.3:
– Definition of the IO revised scheme
– start of implementation of XML input suitable for interfacing FLEUR with Aiida
– Started the implementation of the AiiDA plugin for FLEUR

PALENQUE

• Ongoing work on implementing and polishing geometry optimization routines T1.3.1;
• re-factoring of the stepper mechanism to work both with dynamics and discrete evolution (e.g. geometry optimization) T1.3.1;
• Implementation of the finite-differences calculator for vibrational properties T1.3.1;
• Implementation of the multiple time stepping technique in real and immaginary time for accelerated (Path-Integral) Molecular Dynamics T1.3.1
• Implementation of a Debye crystal calculator and the infrastructure for computing fully anharmonic free-energy differences T1.3.1;
• Preparation of the material for demonstrative tutorials on i-PI which will be held during a CECAM/PSI-k school (EPFL (June 13-17-th) T1.3

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SIESTA
E Artacho, E Anglada, et al. Journal of Physics: Condensed Matter 20 (6), 064208 (2008)
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E Artacho, D Sánchez-Portal, P Ordejón, A Garcia, JM Soler Physica Status Solidi (b) 215 (1), 809-817 (1999)
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WP2

Integrating Needs and Solutions

Two main activities have been launched in the context of WP2:

T2.1 Building the "Observatory to Identify Industrial and Scientific Needs and Challenges"

A number of actions to build the Observatory have been started that will allow to identify the needs of the scientific and industrial community, which is a previous step towards providing specific solutions to these needs.

Links with other networks, projects and groups of influence have been established to make MaX visible to the members of these communities, and open a channel through which they can submit their needs and request for scientific and computational solutions, protocols, resources and eventually services to the MaX community:

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. MaX aims to include 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). MaX joined 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, H2020-FETFLAG. Conversations are ongoing to establish a formal collaboration between MaX and the Graphene Flagship (GF), so that the GF research and industrial teams gain direct access to the services provided by MaX.

Besides, MaX is in process of preparing a set of "introduction kits" with the presentation of the MaX services addressed at different sets of communities:

- Lead users with activities and pilots are already ongoing.
- Interested potential users (e.g. companies using advanced materials, R&D capable groups).
- Local geographical targets (for example, industry vertical association and regional industry districts).

T.2.2 Pilot Cases

The 4 pilot cases defined in the proposal are progressing at good speed. See the attached annex II on each of them.

WP3

The Data Management Plan (D3.1) was delivered to the European Commission on March 1, 2016

T3.2: Data management and the central role of computational workflows

Development of plugins for the Quantum Espresso package as required by the month 12 deliverables D3.2 (EPFL)

- Plugins for the pw.x, ph.x and cp.x codes of the Quantum Espresso (QE) suite of programs have been developed and tested.
- Development of plugins for neb.x, pp.x, projwfc.x and pw2wannier90.x in the QE package are under way.
- Development of plugins for codes codes that interface to leadership codes, such as wannier90 and the Environ computational library.

Development of XML input/output in the QE code and a python interface for the new XML scheme (SISSA)

Development of a plugin for the Yambo code (D3.2) (EPFL&CNR)

- A first version of the Yambo plugin has been developed and tested at EPFL in collaboration with CNR. The functionalities of the plugin include the G0W0 and dielectric function calculations.
- Extension to the full Yambo functionalities is under development.
- The development of a plugin for the Yambo post processors in at the initial development stage.

Preliminary development of a plugin for the Siesta code (D3.2)

- A preliminary version of an AiiDA plugin for the Siesta code has been developed by Victor Garcia Suarez (Uni. Oviedo) during his 3-month visit at EPFL in the group of Prof.Marzari.
- An AiiDA instance has been installed at the BSC to test the forthcoming SIESTA plugin.

Development of Plugins for the Fleur code (D3.2) (Jülich)

- Definition and implementation of an XML based input for FLEUR (done).
- Refactoring and restructuring of the FLEUR output (in progress).
- Development of an AiiDA plugin for the FLEUR code (done, in testing).
- implementation of the parser for FLEUR output in AiiDA (in progress).

T3.2: Data management and the central role of computational workflows

The AiiDA code (and in particular the aiida_core package) have periodic releases with improvements to the engine and additional functionalities. Since month 1, a new version (v.0.5.0) has been released on 17/12/2015. This version includes the possibility of multiple code execution in the same submission script, supports import of XYZ files and van der Waals table in QE calculations. Conversion among pymatgen Molecule and Molecule list to AiiDA data structure has been implemented as well as the possibility to export .zip files and the full support of the Torque scheduler. On the API side it has been included the possibility to add any Django query in group.query, the importer/exporter from the TCOD (Theoretical Crystallography Open Database) and a plugin for the NWChem code.

WP4

T4.1 programming paradigms

- prototype of OpenMP tasking in Quantum Espresso local potential calculation

OpenMP tasks permit to exploit an async scheduling of tasks at runtime. We introduced a new task based implementation in the Vlocpsi of Quantum ESPRESSO in order to improve the scalability in terms of threads. At present, we are benchmarking this new implementaion and, whereas it is advantageous, we will extend that in other parts of the code.

- setup of a benchmarking and validation web-portal

Following the best practice introduced by PRACE, we are building a framework for the collection of benchmarks of material science codes. Our purpose is to collect input data set, building instructions and results of benchmarks of different machines to deliver to the material science community. This collection will be continously updated with new datasets and new results coming from different computer architectures.

- support to the profiling and benchmarking activity of the WP1

The computing centers supported the activity of benchmarking and profiling of the flagship codes made by the personnel of the WP1. The expertise permitted to analyze the codes pointing out the weaknesses and bottlecks requiring optimization and refactoring.

- implementation of the 3D-FFT taskgroup algorithm

Following an external request, we implemented a new data distribution schema that permitted to compute the FFT in QE with a single 3D serial FFT, instead of a distributed parallel FFT.

T4.2 domain specific libraries

- CSCS Sirius domain specific library targeting heterogeneous systems
- Cineca QE FFTXlib targeting homogenous systems

T4.3 Co-design for energy efficient materials science simulations

- Mini-app development

Within the scope of the co-design activities of MAX two mini-app (not originally included in the GA, but adding effort on top of what was already committed) were developed that can be easily ported to new hardware, eliminating all the complexity of the full application but being accurate in reproducing numerical functionalities.

Moreover, the two mini-app do not depend on a specific input data-set but are parameterized to reproduce all possible input cases, giving the opportunity to develop accurate performance models. The two mini-app are related to the linear-algebra and FFT kernels and data-structure of QE. The development of mini-apps has been made possible thanks to another MAX re-factoring activity, regarding the implementation of code independent libraries. In particular for QE two QE independent open source libraries for linear algebra and FFTs kernels were developed that can be re-used for other code. The mini-apps have been presented and discussed with Mont-Blanc that decided to use them in their application on code design and validate them on the Mont-Blanc Excascale architecture as Mont-Blanc / MaX joint collaboration.

WP5

A **parallel website** has been designed and implemented, targeting end-user and public at large scale. A matching graphical image has been developed, with a rich design which is based on the MaX brand guidelines. The respective report (D5.1) was delivered to the European Commission on March, 1, 2016.

T5.1 Industrial outreach

To promote the brand and the website, a set of accompanying material has been created, including a **30 seconds video** presenting the values of new materials in the daily life, a slide deck designed for presenting the MaX services to potential adopters, and info-graphics designed to be printed at wide scale for events and presentations.

A **position paper and initial strategy** was devised and presented at the first MaX plenary session. An initial outline of potential services has been drafted; initial exploration of less traditional models like Kaggle or CrowdAnalytix is being pursued.

An international expert on networked and innovative business models was contacted, Simone Cicero (OSVehicle, OiuShare, Hopen think tank, Open Hardware Conference https://uk.linkedin.com/in/simonecicero) with which we agreed on a collaboration on a research effort for science-based business models, using MaX as a basis for the new **Platform Design Canvas toolkit for business model design**, an evolution of Osterwalder's business model canvas extended for networked and collaborative models.

T5.2 Software-related forums and basic support and

T5.3 Direct users support

The **first working prototype of the user portal** was prepared to gate access to services and documentation for external users. The prototype will provide one-stop access to the services for which the user is enabled (by the portal administrator), to an internal forum and documentation and to direct links for submitting tickets and requests to the projects that collectively form the MaX platform.

WP6

Training and Education events

Education and Training Programme (D6.1) was developed and delivered to the European Commission on March 1 ,2016.

Realized Events

For Max training on material science simulation is of fundamental importance and since the beginning, Max started to contribute to HPC focused training events in Europe promoted be other institutions and projects.
Events dedicated to scientists in the materials field, at different levels, with emphasis on hands-on courses. This training provide technical information and knowledge attracting especially young researchers.

T6.2 University course modules

1) In February 2016 Max (CINECA node) contributed to the master in High Performance Computing (www.mhpc.it) of SISSA/ISAS. MHPC provides skills useful both in the academic and in the industrial field, like technical and software development. MaX contributed in advanced training in programming in intel accelerators platforms.

T6.1 Specific Training Workshops/Courses

2) In January 2016 Max (CINECA node) contributed to the "Joint MCC-UKCP-EPCC Workshop on *ab initio* Periodic Codes" cosponsored by PRACE PATC (https://eventbooking.stfc.ac.uk/news-events/joint-mcc-ukcp-epcc-workshop). The workshop was directed to advanced users of *ab initio* codes in HPC computers. The training offered by Max dealt on Advanced functionalities and tutorial on the flagship code Quantum-Espresso.

3) From January 16 to 28, 2016, the ICTP hosted the MaX event "Linear Response workshop 2016", organized jointly together with SISSA (http://www.quantum-espresso.org/resources/advanced-quantum-espresso-developers-meeting-linear-response/). The event was aimed at coordinating effort and defining new milestones for the development and improvement of codes in the quantum-ESPRESSO package. The particular focus was on applications of density-functional perturbation theory, an approach to the calculation of phonons and other linear properties within the general DFT framework. This workshop has seen the participation of about 40 developers of quantum-ESPRESSO from all over Europe (mainly Italy, France, UK, Switzerland) as well as from the U.S.

4) A tutorial on AiiDA (http://nccr-marvel.ch/en/events/aiida-tutorial-coding-days) had been held on November 2 and 3, 2015 at EPFL (Lausanne, Switzerland); this tutorial was followed, from November 4 to 6, by three days on coding for interested plugin developers. The tutorial and coding days were attended by developers of the MaX flagship codes and Aiida plugins were designed.

MaX offered Materials Science modules within the following courses

5) A Python for computational science' organized by MaX (CNR and CINECA teams) held in Modena from 25 to 27 January 2016. Materials science students attended the course and during the course, examples on the usefulness and versatility of the Python language as post processing tool for scientific problems in material science were illustrated.

6) A course on HPC Numerical Libraries (http://hpc.cineca.it/content/hpc-numerical-libraries-0) held at CINECA, Bologna on 26-28 April 2016. In this course, some of the most important numerical libraries of HPC will be presented. In this context, MaX will offer a "materials science" module by illustrating specific libraries particularly suitable in algorithms, which are common in materials science codes, as for instance FFT tailored on purpose for plane waves code.

Programmed Events

Events dedicated to scientists in the materials field, at different levels, with emphasis on hands-on courses. This training provide technical information and knowledge attracting especially young researchers.

1) The Cineca MaX node is involved in prepare with PRACE PATC a material science extreme scale simulation workshop to be held in Q4 2016 or Q1 2017.

Together with SISSA, ICTP has coordinated efforts to find partnerships and collect additional funding for the organization of two events in 2017. In particular:

2) a Workshop on "High-Performance & High-Throughput Materials Simulations using QUANTUM ESPRESSO" is planned at ICTP in January 2017. The event has already received confirmed co-sponsorships by the MARVEL center on Computational Design and Discovery of Novel Materials (Switzerland), the Centre Européen de Calcul Atomique et Moléculaire (CECAM) and the E-CAM Centre of Excellence.

3) A similar effort is on-going for the MaX conference "The Materials Design Ecosystem at the Exascale: High-Performance and High-Throughput Computing" which is planned for the end of the MaX project (November/December 2017).

4) The MaX developers team of FLEUR will organize with the support of the CoE an hands-on tutorial for new users as done in the past within the CECAM/PSI-K networks (http://www.cecam.org/workshop-1035.html) and a workshop dedicated to more experienced researcher and developers.

5) The MaX developers team of YAMBO (CNR) will organize an hands-on workshop in the same spirit of the workshop: Excitations in Realistic Materials using Yambo on Massively Parallel Architectures (http://www.cecam.org/workshop-1149.html). This workshop will consists in theoretical lectures on Many Body Perturbation Theory, technical lectures on the parallel algorithms of the code and an hands-on tutorial particularly focused on the exploitation of the code in massively parallel, distributed memory architecture. During this workshop, CINECA will offer a dedicated lecture on trends in parallel computing. The workshop will be held in Modena or Lausanne in spring 2017.

6)A Siesta school on efficient DFT calculations using atomic orbitals will be organized by MaX partners (BSC and ICN2) at Barcelona Supercomputing Center in winter 2017. The target would be to offer an extended how-to of the use of Siesta, both for beginners and advanced users.

7) A MARVEL/MaX/Psi-k Tutorial on high-throughput computations: general methods and applications using AiiDA (http://nccr-marvel.ch/en/events/aiida-tutorial-june-2016) will be held on June 22 to 24, 2016 at EPFL (Lausanne, Switzerland). The programme includes a tutorial on the Aiida code, and three invited highlighted talks from expert in the field of high throughput computations.

MaX will offer Materials Science modules within the following courses

8)In the next PDC Summer School: Introduction to High Performance Computing (http://agenda.albanova.se/conferenceDisplay.py?confId=5012) organized by the PDC Center for High Performance Computing and the KTH School of Computer Science and Communication (CSC) in August 2016 in KTH main campus in Stockholm, MaX members will illustrate case studies in Materials Science and will offer projects based on materials science as part of the project work.

9) MaX will offer a “materials science” module by illustrating specific libraries particularly suitable and extensively used in materials science codes in the Introductory School on Parallel Programming and Parallel Architecture for High-Performance Computing to be held at ICPT Trieste in October 2016 (http://indico.ictp.it/event/7659/).

10) In early 2018, MaX will organize at BSC in Barcelona a developer workshop focused on new programming paradigms and addressing the memory hierarchy challenge. The concept would be to use work that has been done during the MaX developments as base for examples in the context of materials science codes, presenting also lessons learned and best practices. The target audience would be material science code developers, but this could also be extended to scientific computing in general, in connection to other CoEs.

In addition to the integrated code-specific and HPC-specific workshops and courses, an school will be offered to support new methods and software developments produced in the CoE:

11) A PRACE/MaX school will be organized in collaboration by CINECA and CSCS focusing on several of the main codes used by the materials science community (namely, the MaX flagship codes Quantum Espresso, Siesta, Yambo, Fleur), introducing their architecture and usage. The course will explain how the codes exploit petascale systems, targeting in particular to PRACE Tier 0 systems, and how they are moving to the exascale era, with specific attention to hybrid, accelerated architectures. Hands-on activities will be proposed to let the attendees familiarise with the codes and their optimal usage on HPC systems. The course will address in particular the MaX community, more specifically the users of the selected codes and the software developers starting contributing to those codes with new components and functionalities targeting the support of novel architectures and the performance and scalability improvement. The two- or three-days course will be held at CINECA in the period November-December 2016. Lecturers will be provided by the involved PRACE partners and by the MAX project members.

Beside these dedicated schools on flagship codes, developers of MaX codes will offer training in computational materials science schools as

12) College on Multiscale Computation Modeling of Materials for Energy Applications, held at ICTP Trieste 4-15 July 2016 sponsored by PSIK and ICTP (http://indico.ictp.it/event/7656/): the EPFL MaX partner will offer a training on the Aiida platform.

13) CECAM/PSIK/CCP9 Graduate School in Electronic Structure Methods, Daresbury 5-9 September 2016 (http://www.cecam.org/workshop-0-1265.html). SISSA and CNR MaX partners will offer hands-on tutorials on flagship codes Quantum Espresso and Yambo.

14) A Winter School in Multiscale Modeling will be organized in Stockholm by KTH in Winter 2016/2017 (see http://sese.nu/multiscale-2014/ for a past event). KTH MaX partner will offer a module on exascale perspective.

T6.2 University Course Module

15) As already done in February 2016 MaX will contribute to modules of the joint SISSA/ICTP Master in High-Performance Computing (MHPC) (http://mhpc.it). Academic year 2016-2017 Applications deadline 6 July 2016.

16) MaX (Jülich team) will contribute to the Master Course at the German Research School for Simulation Sciences offering lectures on Electronic Structure Theory, with a focus on HPC applications for materials science.

17) MaX (CNR team) will complement a University course on computational Physics at the University of Modena and Reggio Emilia with lectures on HPC and tutorials on computational materials science providing hands-on on flagship codes.

Massive Open Online Courses

Massive Open Online Course will be developed by MaX in collaboration with ICT and EPFL:

Modules of the Master in HPC program related to Exascale and Material Science will be recorded and made available through the MaX portal. Recording and editing for preparation of video lectures will be also done in occasion of the Advanced Workshop on High-Performance & High-Throughput Materials Simulations using QUANTUM ESPRESSO, (January 16-28 2017), and possibly in Jülich for the Master Course at the German Research School for Simulation Sciences. In occasion of seminars of interest for the CoE, the lectures at CNR, EPFL and ICTP will be recorded in order to collect a series of video lectures on the mode of Marvel distinguished lectures (http://nccr-marvel.ch/en/events/marvel-distinguished-lecture-ceder) and made available on the MaX website.

T6.3 Training through research in CoE laboratories

"Training through research" in the CoE labs will be coordinated by ICN2 and CNR. Experience shows that this is an extremely powerful instrument both for industrial researchers and for academic researchers/PhD students. Successful examples for such activities are the collaborations of Total and Toyota with the partner CNR. Marie Skłodowska Curie networks will support the academic users.

Training courses will be organized through existing Marie Skłodowska Curie networks. To form an own network MaX will promote an application for the next Horizon 2020 - MSCA calls. MaX will also offer internships of short/medium duration to PhD students willing to gain experience with the MaX flagship codes.