Position Paper: The Commercial interactions within the MaX Centre of Excellence for computational material design

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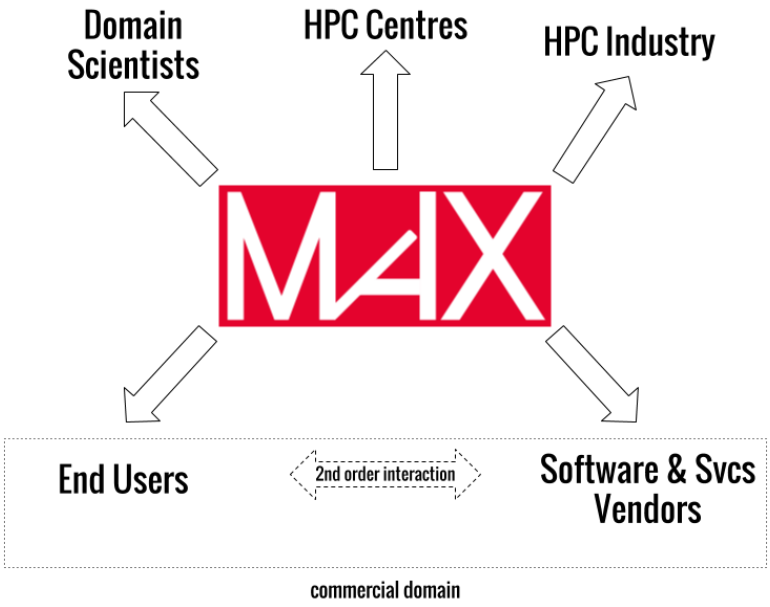
MaX (MAterials design at the eXascale) is a user-driven European Centre of Excellence (ECoE) established to support developers and end-users in materials simulations, design and discovery. MaX focuses in enabling the best use and evolution of HPC technologies by creating an ecosystem of knowledge, capabilities, applications, data workflows, analytic tools and user-oriented services. In addition to creating a best-in-class research environment, MaX addresses for the first time the hurdles of bringing the results of this research directly towards end-users and commercial actors like software vendors, system integrators and service companies. In fact, while computational modelling has demonstrated in many ways to be able to transform the way we understand, and ultimately design and manufacture materials, some of these models have yet to become pervasive in industry. This has been recognized as one of the biggest hurdle, as mentioned in many EU research reports[1]: " However, this can only be exploited if complete materials model systems are created and when these are complemented by highly skilled actors who translate industrial problems into cases to be simulated with materials models."

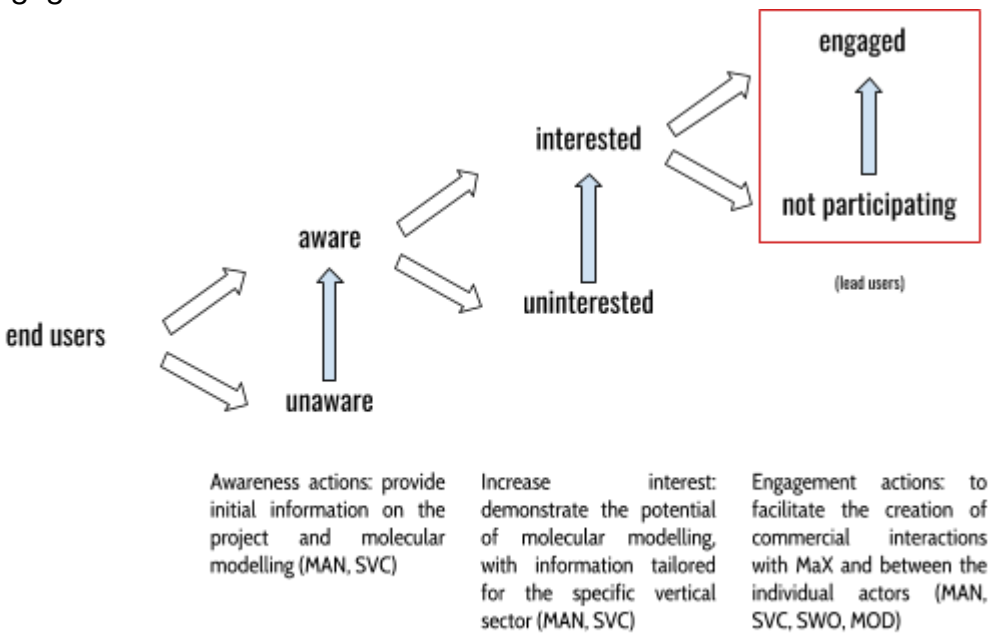


Taking into account the actor taxonomy already explored in the MaX position paper, the commercial side will focus on providing services and tools to the following groups:

[1] "Materials Modelling: Where do we want to go?" EU Directorate-General for Research and Innovation, Key Enabling Technologies (NMPB)

- **MAN:** manufacturing and engineering industries ("the end-users")
- **SWO:** commercial software owners (who sell materials models and software tools directly or indirectly to end-users)
- **MOD:** materials modellers (academic and industrial model developers)
- **SVC:** service providers (computational and storage capability providers, validation, IPR notary services, workflow plan and execution, optimization)

Initially, MAX will focus on a set of activities designed to accelerate the take-up of MAX results by both groups, and in the second phase to promote actively the communication between groups to facilitate any possible commercial interaction. MAX will perform (in addition to the scientific and technical production) a set of actions designed to facilitate take-up, based on a "ladder model" of commercial engagement:



We are certainly not the first group to show the existence of different level of engagement in the industrial adoption of molecular modelling. For example, the WTEC Panel Report on applications of molecular and materials modelling indicated that "Management and employees may view these activities as ... a luxury that can be eliminated in times of cutbacks. Management and old-line employees often still reject or suspect the value of molecularly based modeling… when people find a tool or skill or service that can make a difference, they seek it out. Increasingly, they are familiar with the usefulness of these methods, [and] they expect that these capabilities will be available as a matter of routine, just as they expect to have gas chromatographs or other analytical equipment."

MAX is in this sense the first project to provide, in a single contact point, the entire spectrum of services and knowledge necessary to bring commercial actors up the entire value ladder.

The MAX commercial valorization strategy takes advantage and leverage the same MAX key actions mentioned in the MAX position paper:

- Implementing a **Sustainable Programming Platform:** this is valuable for software companies interested in taking advantage of the MaX code base; it will reduce substantially the cost and effort necessary for take-up within existing commercial codes, adding functionality without resorting to long development efforts and post-integration validation;

- Building a **Dynamic Data Framework** to manage the automation of high-throughput calculations, automatic data storage, workflows interchange: this will be of interest not only for software developers (reducing data transfer and integration costs) but for turning MaX into an extended platform for other codes as well, increasing its value for every adopter;
- Promoting the **Exascale Transition Enabling Action** through the development of novel algorithms, domain-specific libraries, in-memory data management, and software/hardware co-design: the MaX platform will scale from small, private-cloud like environment that may be suitable for internal development and exploration to exascale-level with the same set of tools and technologies. This will facilitate market exploitation by external actors, that will see MaX as a "safe" platform independently of problem scale.
- Establishing the **User Needs and Solutions Integrating Protocol** by aligning the technological offer with leading end-users requirements: this will facilitate the adoption by SMEs and other vertical sector companies that may need specific extensions or adaptation for their applications;
- Developing a **Catalogue of Services**: this will facilitate not only commercial exploitation by end users, but will also provide a good start for external actors that may want to complement MaX-provided services;
- Contributing to the diffusion of material simulations by addressing the skills gap through an integrated offer of **Training and Education**: this will help third party in finding competences and skilled people already trained in the basis of molecular modelling and the MaX toolset.

The initial activity will center on the creation of a end-user specific website, designed to address each of the four main actor groups; this will be complemented with a set of specific actions designed to help the transitions unaware → aware; uninterested → interested and not active → engaged. Each action will be customised for each actor group, and a parallel measurement effort will be performed to guarantee the maximum efficiency from each action. As the actions themselves are expected to take a substantial time to provide a visible conversion, we will focus on the so called "lead users" (from "interested" to "engaged"), that is users that are already using molecular modelling, and for which the MAX proposition will be explicitly promoted.

The second part of the project will see the introduction of a novel model, called "Quantum-as-a-service", or QaaS. It is envisioned a set of "universal" (or self-adaptive) Virtual Machines that can be executed both on HPC infrastructures belonging to the customer, MaX partners or on external cloud service like Amazon AWS or Microsoft Azure. It will allow to easily access the whole set of MAX flagship codes in an easy-to-use package, reducing the complexity of adoption and the initial hurdles for creating a stable and high quality platform for running materials modelling simulation.

MAX will help bring the potential of molecular modelling to the broadest possible public and help EU companies in taking advantage of the European research excellence and turning it into new materials, new products and new opportunities.

MAX is one of the eight 'European Centres of Excellence for HPC applications' supported by the EU under its H2020 e-INFRA-2015 call, GA: 676598. The MAX consortium includes 5 research institutions: CNR Modena, SISSA Trieste, ICN2 Barcelona, FZ Jülich, EPFL Lausanne. 5 supercomputing centres: CINECA Bologna, ETH/CSCS Zürich/ Lugano, FZ Jülich, KTH Stockholm , BSC Barcelona. 1 global research & education institution: ICTP Trieste. 2 SME business partners in hw and open source technologies: E4 Computer Engineering Scandiano (Reggio Emilia), CloudWeavers London.