D10.2

Draft business plan: preliminary exploitation strategy

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Contents

1. Executive Summary

This report discusses a preliminary business plan to assess the sustainability of the activities of the MaX European Centre of Excellence beyond the current H2020 funding scheme.
The first part summarizes the potential market segmentation and size for commercial exploitation of MaX results and of the related activities and competence of its partners, with reference to both the industrial and the academic and public sectors. The possible value components and the definition of services are analyzed on the basis of the current literature, as well as the experience and data collected during MaX operation. A set of commercial activities are identified, essentially based on consultancy and services at various different levels, that are compatible with the open-source nature of MaX codes and have a demonstrated success record in the activities of the CoE and its partners.
The second part examines the legal instruments that could be adopted to set up MaX as a legal entity, taking into account the interests and expected constraints of MaX partner institutions, and presents a draft business plan on which the sustainability of the new legal entity can be assessed. Finally, an economic and financial plan is drafted for three-year development of the activities, which relies on a realistic estimate of revenue and cost streams based on data provided by MaX partners for the last two years.
The main conclusion is that a MaX entity essentially based on commercial activities would be sustainable beyond the end of the current H2020 funding period. Further details, and the interest and role of the different MaX partners in this initiative, will have to be assessed in the next one to two years.

2. Introduction

MaX is a European Centre of Excellence for High Performance Computing (HPC) focused on the domain of materials simulation, modeling and design. Its mission centers on the best performance and evolution of quantum electronic-structure based codes towards extreme computing at the exascale and beyond, and on the convergence with high throughput and high performance data analytics. A major effort is devoted to services, training and dissemination activities to support and expand the large users community of the present codes, strengthen the European ecosystem and the impact of MaX research in industry and academia.
At the end of its first three-years phase (2015-2018), MaX presented a report where a general exploitation strategy of MaX results was already analyzed with special reference to the potential market size and the individual value components [1]. It was then pointed out that most of the core research activities of MaX, aimed at extreme computing and frontier innovation, require long term investments and funding that exceed what could be sustained by commercial activities alone. Such long term activities, vital for the future of European science and technology, still

need substantial long-term public funding in order to maintain global leadership and ensure economic and societal impact.
In the same report, it was emphasized [1] that a number of activities and services delivered by MaX to its users had a clear potential to bring revenues that could make the Centre self-sustainable in the medium term, albeit with a more limited range of activities, even in the absence of the major public funding that made it possible sofar.
The present work aims at updating and extending this latter analysis, as requested by the EC, by analyzing the legal instruments and the economic and financial strategies that could be adopted to set up MaX as a self-sustainable legal entity essentially based on commercial activities. Public funding deriving from national and international projects was intentionally included only at a marginal level at this stage. A draft business plan, a realistic estimate of the revenue and cost streams, and an economic and financial plan for the first three years of activities, are presented to assess this hypothesis.

3. Potential market size

The first part of this document is based on estimates of the potential market size, users and value components that were obtained in the first phase of the MAX European Centre of Excellence (CoE) [1]. It is updated taking into account more recent data, as well as an updated scenario of possible business models and sustainability for materials modelling software reported in recent papers by Goldbeck 2018 [2] and by the European Materials Modelling Council (EMMC) [3].

Based on the data collected about the activities of the MAX CoE and of MAX partners, as well as the current literature, we broadly classify the "users" of the current MAX codes into academia, industry and a much smaller presence of government actors (for the purpose of this analysis, the latter is aggregated with academia). A further useful distinction is between entry level and experienced users -- a distinction that has a significant impact on the kind of services that can be offered and their take-up probability.

3.1 Industry

MAX users in industry include:

- Commercial developers of materials simulation software (often named independent software vendors, ISV)

- Manufacturers (end users): This group represents the end-users of materials modelling in small and large European manufacturing industry. It covers many industrial sectors and materials categories, from consumer goods to industrial chemicals, from polymers to alloys etc.

In addition there are now companies in the market, sometimes named "translators" [4], which are bridging from software owners or vendors to end users. They start from an industrial

problem and identify a workflow for its solution by using materials modelling. Their activity includes the identification of all quality attributes, or at least the most important ones, within the language of the context of the technical industrial problem. This includes non-technical cost measures, like the influence of the solution on the pricing of a final product, and time to market. In practice, these companies are mostly firms acting as consultants for large manufacturers in the Materials Design process. The category also includes some vertical groups, like engineering specialists that "package" simulation workflows in custom software systems [5]. While the underlying simulation code is open source, the packaging provides an easy-to-use interface that automates most parameter building and post-processing.

There is very limited amount of data on the size of the market for quantum materials simulation software, in part owing to the very small size of the market itself that limits the interest of consulting companies in performing such measurements. We refer essentially to the business plan produced in first phase of MAX by C. Daffara [1] (and references therein) and to the only analysis with a clear methodology from Goldbeck Consulting [6].

Concerning the number of ISV companies, Goldbeck reports that even if new software companies have appeared on the market, a consolidation among the largest vendors acquiring smaller players gives an overall flat market, with the number of vendors being mostly static around 40 players. Our evaluation, including a list of software vendors [1], and Goldbeck's analysis [6] are within the same order of magnitude. We thus conclude that the overall market for software integration services can be estimated within 30 and 40 potential adopters, [7] with aggregate revenues around 100M$.

Concerning industrial end users, Ref. [1] provides an economics-based estimate concluding that in Europe the potential market of manufacturing companies with ongoing modeling activities, thus potential MAX users, is around 600 large and medium companies and 1500 small companies. This estimate is consistent with the results of the EMMC [8] where the group identified 1500 potential stakeholders (a number that includes research and academic entities). The market report by Goldbeck Consulting [9] confirms the core-user communities identified in [1]:

- Pharmaceutical and biotechnology
    - Discovery ("Life Science")
    - Development ("Materials Science", Analytical Chemistry, Process Chemistry)
- Chemicals industry
- Materials development for a wide range of products, such as automotive, aerospace, and other transport applications, consumer packaged goods (home and personal care, foods), adhesives, packaging, plastics etc.
- Electronic devices.

The latest analysis of the market elaborated by Adamovic 2016 [8] concludes that, as shown in Figure 1, automotive (31%) and chemical (27%) applications combined represent more than half of the total the primary field of application of materials modelling software, followed by energy (12%), metallurgical (7%) with aerospace representing 6%. Within the automotive applications, the dominant secondary application is metallurgical (36%), followed by chemical applications (29%). Within the primary chemical applications, energy represents 24% followed by metallurgy (12%) and electronic applications (10%). Other applications mentioned in the survey include composites, polymers, fuel cells, coatings, optical coatings, photovoltaics, formulations, detergents, complex fluids, nano and microfluidics, memory devices, magnetic data storage, spintronics, organic electronics, adsorption engineering for environmental applications, water (environment), medical engineering, cosmetics, consumer care, construction, radiation protection, packaging, pulp and paper.

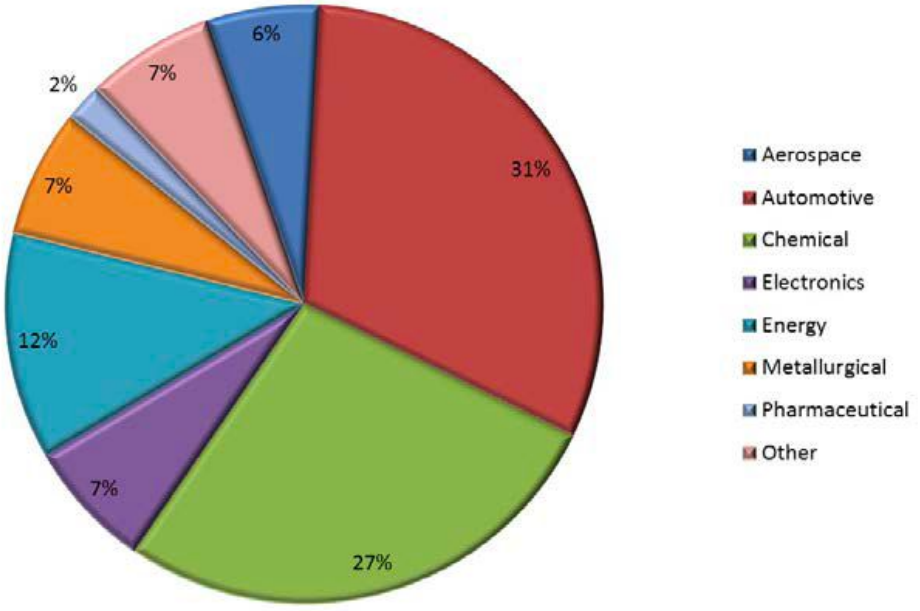

Fig.1 Primary field of application of materials modeling software (Source: Adamovic 2016 [8]).

To further validate the market size estimate in industry, Ref. 1 performed an analysis of the job postings in the CCL list, the online job marketplace Indeed.com and Linkedin jobseek. The CCL lists 166 job posting in the years 2017-2018; the vast majority are related to public-private partnerships with universities, while the remainder are fill-in positions in large companies like BASF or Ely-Lilly. Indeed.com lists 367 jobs in the computational chemistry category, with nearly 50% of the vacancies coming from large companies, with the rest coming from universities and research centres. Linkedin has a much smaller list of open jobs, with only 70 listed in both molecular modelling and computational chemistry (and synonyms) with 13 vacancies coming from software development companies. This analysis leads us to believe that the original focus of MaX - with equal importance to small, medium and large companies - needs to be adjusted, with a much stronger importance towards medium and large industrial users, in addition to academic users.

Concerning the size of the market, data from from Goldbeck 2017 [9] show that:

• For pharma and biotech, the combined R&D spend is about $100bn, and the spending on scientific modelling and simulation software is about $100m.

• In the Chemicals/Materials industry the R&D spending is about $50bn, and the molecular modelling software market for chemicals and materials is about $50m.

• The number of users of scientific software such as molecular modelling in chemicals/materials is in the range of a few thousand in industry and a few tens of thousands in total.

Ref. [2] introduces segmentation of materials modelling software market along two other dimensions:

1. By considering the position in the value chain where materials modelling is used.

2. By the type of modelling, in particular data-based versus physics-based modelling and for the latter by the entity type described (electronic, atomistic, mesoscopic and continuum).

The two dimensions are actually not completely independent, since at least currently there is more use of continuum models downstream, as Figure 2 illustrates.

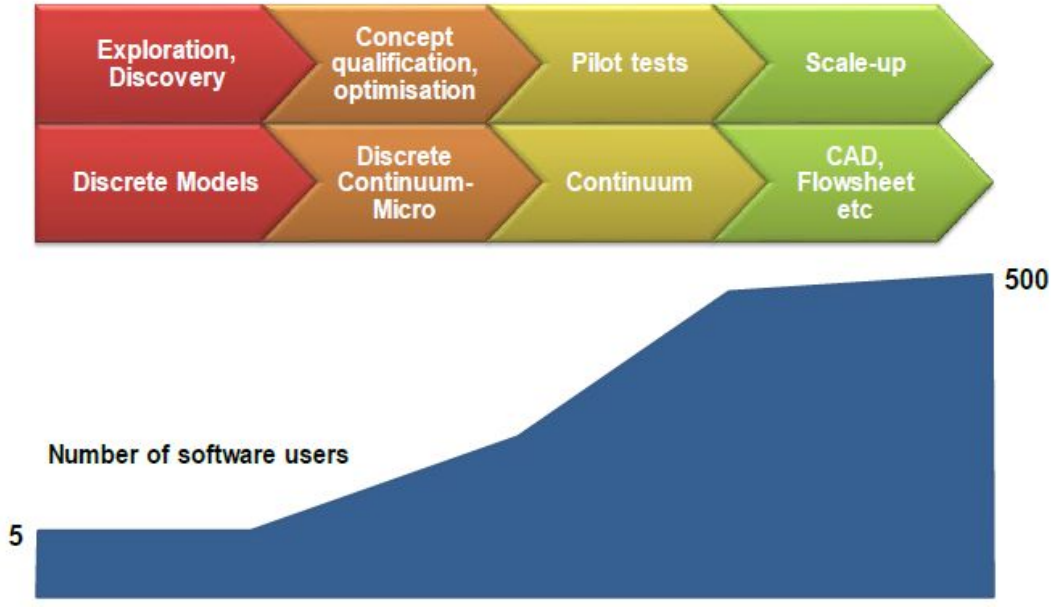

Figure 2. Mapping of Product Value Chain (exploration to scale-up), typical model used (discrete to CAD), and number of software users at a large company. (Source: Goldbeck 2018 [2]).

1. Market segmentation by value chain

The development and engineering sector representing the design *with* a given material is far larger than the materials research and design sector where the target is to develop *the* material itself. There are estimates from market research organisations for the size of the Computer-Aided Engineering (CAE) market, which roughly represents the former (design *with* the material) but will also include a lot of design software which is strictly outside of materials

modelling. The total market size is about $4bn with a CAGR of about 11%. From public reports of companies which represents "modelling *with* materials" we can deduce that the total market for materials modelling software in the downstream sector is more than $1bn.

A rough estimate of the market size for materials modelling software in the "design *the* material" sector is in the range of $100m, i.e. about a factor of 10 smaller than the downstream sector. This estimate is based on revenues and number of employees in relevant software companies.

2. Market segmentation by type of modelling

The Continuum Materials Modelling Market is a large fraction of the CAE market (which also includes some more design type and data management applications). It is estimated in the region of at least €1bn which makes it an order of magnitude larger than the discrete modelling market.

The Discrete Modelling market is estimated to be in the region of € 100m. The share within that market of electronic atomistic and mesoscopic modelling is not documented, however anecdotal evidence, backed up by hard evidence such as number of software codes and companies, number of documented users etc., suggests that electronic models make up the largest part, followed by atomistic and then mesoscopic modelling.

This market segmentation is represented in Figure 3.

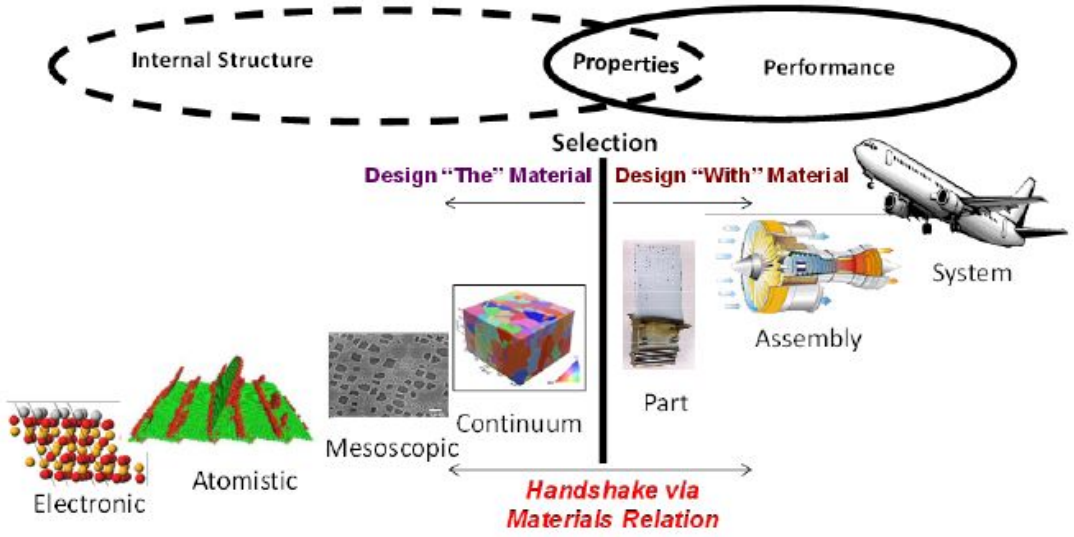

Figure 3: Segmentation of the Materials and Engineering Modelling market by type of modelling: designing *the* material on the left, and designing the product *with* the material on the right (Source: Goldbeck 2018, Courtesy of Granta Design [2]).

Note that here the definition of the types of modelling is the one proposed by the EMMC [2, 8]: hence, "electronic modeling" refers to quantum-mechanical electronic-structure based modeling. The main strength of MAX codes is precisely in such electronic modeling and its interfaces to atomistic modeling.

Two key factors related to the dynamics of the materials modelling software market are:

• The continuum materials modelling market is relatively mature in the case of engineering focussed applications (design *with* the material), where the focus has been on large scale integration of CAE, CFD etc (i.e. integrating all types of 'physics'), CAD, PLM and even asset management. However, there are many small and relatively fast-growing companies representing the continuum modelling of the material. Some of these companies have also been acquired by the global CAE/CAD/PLM corporations.

• The discrete materials modelling market went through a period of consolidation in the 1990s, followed again by new companies and ventures starting up since then. Some companies have been taken over by large modelling and design corporations but there remain a significant number of smaller players and start-ups.

Considering all entries of the survey performed by Adamovic 2016 [8], it comes out that the dominant models used across all application areas are the so-called "electronic models" (34%) followed by mesoscopic (28%) and atomistic (22%). Among the contributors to this survey, 14% used predominantly continuum models. Users focusing primarily on "electronic models" employ atomistic models as secondary tool and to a much lesser extent mesoscopic and continuum models. Users applying primarily atomistic models rely mostly on mesoscopic and continuum models as additional tools.

Considering only industrial users, the largest application is mesoscopic (32%), followed by "electronic" (24%), continuum (20%) and atomistic (18%). In other words, industrial users exhibit a stronger emphasis on mesoscopic and continuum models when compared with the entire set of users of the survey. This means that academic researchers employ more electronic structure methods and less mesoscopic and continue models. However, overall the distribution between e/a/m/c among the industrial users is not dramatically different from the entire group.

These results are shown in Fig. 4.

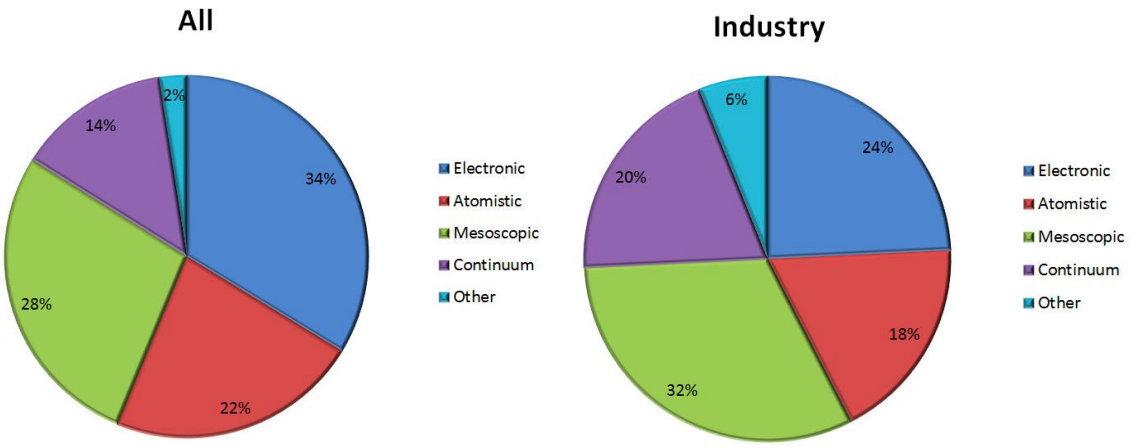

Fig.4: Models used in all application areas by all users (left) and all industrial users (right) of the EMMC survey (Source: Ref. [8])

While the number of companies selling software for molecular modelling and chemical simulation remains small (and heavily concentrated) the number of potential end users and the related market is much greater (the corresponding overall R&D spending is much larger). Analyzing the market shows that adoption is concentrated on one very large vendor (Biovia/Accelrys) with many smaller vendors; Biovia has more than 50% of the market share, but only 5% of the adopting users - since the majority of users implement and use only open source platforms for their scientific and simulation use. This means that the potential market for services based on our open source experience and the codes themselves could be large enough to sustain MaX as a commercial entity.

3.2 Academic users

A similar economics-based estimate of the potential market for academic users is extremely difficult because most of the activities are not based on a for-fee exchange and are not covered by analysts. The estimate is thus necessarily based on the current users base of MAX codes. In general, use does not occur through registered access, so we refer to the users of the services operated by MAX in its first phase and the publications citing the code. (Note that data for services do not include two of the present flagship codes: CP2K and BigDFT, which were not part of MaX in its first phase.) Such data show

- users: 470 users per year of MAX-operated advanced services (including software support, consulting, training) and about 9500 users per year of basic support services: forum/mailing list subscribers, unique download of code releases (MAX data, Feb 2017). Further analysis shows that approximately 95% of the users is from academic or governmental institutions.
- citations: the number of publications explicitly citing the use of MAX codes is 4633 so far in the year 2019 (was 4249 in 2018, and 3918 in 2017, with an average yearly growth of 9.5%; data from Google Scholar, same search criteria as in Ref. [10]).

MAX has now in place a set of dissemination actions, also in collaboration with FocusCoE, which could expand significantly the user base.

4. Business model

4.1 Identification of value components

The components that form a business model are value architecture (revolving around organizational resources and capabilities as well as their configurations); value network (representing the external arrangements which revolve around the communication and collaboration the organization needs and conducts with other businesses in its value chain or value network in order to be able to offer its products and/or services), and value finance

(revolving around the financial arrangements the business organization conducts for its value proposition and value architecture). The value proposition component is typically depicted through the inclusion of all core products and/or services.

The first step is the identification of the available resources, i.e. the set of tangible and intangible resources that can be assembled or used to provide value to customers. The business model produced in the first phase of MAX [1] classifies the potential value offering within three classes:

- knowledge: the expertise and experience within the consortium, extending also beyond codes,

- code: the collection of the MAX codes and any ancillary and supporting software and documentation, and

- execution capabilities: the set of material and immaterial resources, including licensing agreements, that are necessary to use the codes and obtain a usable result.

This classification is still useful to design potential business models, and we can easily show that it is at least capable of mapping all the current service activities of MAX as listed in Table 1.

SERVICES	description, examples	WP	target users			
			public institutions	large projects, large-scale infra structure	large industrial users	SMEs, small research groups
1. High-level consultancy	° support for the users on the most suitable code/application and on the best choice of the parameters and configuration in order to obtain the best performances in calculations; ° ad-hoc solutions for users, possibly comprising code development; ° dedicated consulting and support for the development of new features in MaX codes	WP1 to WP7	xxx	xxx	xxx	xxx
2. Turn-key materials solution	Turn-key solutions for the automatic computation of advanced materials properties: ° computation of the DFT ground state, relaxed crystal structures, electronic band structures, equation of states etc with MaX codes; ° development of tailored workflows: solutions from single accurate calculations to intensive high-throughput simulations that use the MaX codes and algorithms and are able to scale efficiently on available pre-exascale HPC machines.	WP5, WP7	x	xx	xxx	xx
3. Simulations on premises and in the cloud	° use of AiiDA lab, a cloud platform based on jupyter and jupyterhub AiiDA and most of the MaX flagship codes ° OpenStack installation and viable model for internal company use (including technical, support and possibly legal aspects) ° Use of Quantum Mobile— a VirtualBox machine that comes with AiiDA and a set of commonly used quantum codes preinstalled.	WP5, WP7	x	xx	xxx	xx

4. Training	° workshops and schools on HPC applications in material sciences ° contributions for University courses (undergrad and graduate level) ° training through research in MaX labs ° specific training activities for industrial end-users	WP8	xxx	xxx	xxx	xxx
5. Container technology for HPC systems	° exploiting container technologies for MaX codes on HPC systems (docker, shifter, singularity)	WP5, WP7	xx	xx	xxx	xxx
6. Help desk	° Evaluation of the performance of MaX codes (and some other codes in the materials science domain) on different architectures; ° Analysis of a MaX code that behaves differently from documentation (e.g. algorithm not converging); ° Bug-fixing of problems due to a specific code implementation, e.g. GPU, MPI, OpenMP versions; ° Selection of best code parameters to minimise the time to solution; support in the usage of different releases of MaX codes (user guidance about new vs deprecated features).	WP7	xxx	xx	x	xxx
		*number of x indicates relative uptake (past and current) by different target users				

Table 1. Services that are currently offered by the MaX CoE.

Tentative models of interest for MaX, referring to the above classes, can be mapped on the MaX services of Table 1 as follows:

- Knowledge:
  - specific training activities for industrial end-users
  - training through research in the CoE labs
  - contributions for University courses (undergraduate and graduate level)
  - workshops and schools on HPC applications in computational material sciences
- Knowledge+Code:
  - support for the users on the most suitable code/application and on the best choice of the parameters and configuration to run calculations in order to obtain the best performances
  - ad-hoc solutions for users, possibly comprising code development
  - dedicated consulting and support for the development of new features in MAX codes
  - turn-key solutions for the automatic computation of advanced materials properties: Computation of the DFT ground state, relaxed crystal structures, electronic band structures, equation of states and more with MAX codes.
  - turn-key solutions for tailored workflows: solutions from single accurate calculations to intensive high-throughput simulations that use the MAX codes and algorithms and able to scale efficiently on available pre-exascale HPC machines.

- OpenStack installation and viable model for internal company use (including technical, support and possibly legal aspects)
- exploiting container technologies for MAX codes on HPC systems (docker, shifter, singularity)
- evaluation of the performance of MAX codes (and some other codes in the materials science domain) on different architectures
- analysis of a MAX code that behaves differently from documentation (e.g. algorithm not converging)
- bug-fixing of problems due to a specific code implementation, e.g. GPU, MPI, OpenMP versions
- selection of the best code parameters to minimise the time to solution; support in the usage of different releases of MAX codes (user guidance about new vs deprecated features).

- Code+Execution:
  - use of AiiDA lab, a cloud platform based on jupyter and jupyterhub AiiDA and most of the MAX flagship codes
  - use of Quantum Mobile— a VirtualBox machine that comes with AiiDA and a set of commonly used quantum codes preinstalled.

In the following we discuss the value propositions that result from the remaining combinations:

● Code. For code, the relevant value proposition is mediated by the licensing, that for all MAX codes is an open source license. In a traditional (proprietary) licensing environment, the value proposition would be based on a licensing agreement; to make a relevant example, a proprietary software vendor interested in distributing a software component would license it and pay a per-unit or a yearly rate. In the open source world this would be possible only for the model known as dual licensing, an arrangement that is currently not used by codes within the MAX platform.

A different approach is helping adopters in integrating some or all the MAX codes within a proprietary environment, or an open source environment with an incompatible open source license. Since the MAX codes are under an open source license, this integration raises some additional difficulties related to license compatibility and in general license compliance; this model was not predicted in the original service model of MAX, but was then demonstrated as one of the requested support activities, and has led to the signature of a substantial contract with the US commercial software developer Schrödinger, that requested support for integrating one of MAX codes (Quantum ESPRESSO) within their modelling and simulation suite; similar opportunities are also forthcoming for other MAX codes.

● Execution. Pure execution is not perceived to be a substantial opportunity for MAX, as it would be no different from leveraging a HPC provider, without taking advantage of the specific capabilities of the MAX partners.

● Knowledge+Execution. We consider this combination marginal, as it would not be specific to any of the MAX codes

● Knowledge+code+execution, finally, can simply be interpreted as MAX as a single-stop-shop where the end user would be able to get training, support and execution of workloads as well. It would be equivalent to the superposition of already described models, with no additional value added.

A final comment concerns the Code+Execution combination. This combination can be considered equivalent to the general concept of SaaS (Software as a Service). Since MAX would be in the position of offering both the code and the services, we estimate this to be a potentially important model, despite the negative aspect that this may be implicitly competing with the execution resources offered by some of the consortium members. A possible model, named QaaS (Quantum-as-a-Service), was then drafted in the first phase of MAX, based on the plausible evolution of the market and the overall interest expressed by some of the industry contacts to which a pre-release of the service proposition was presented. Ref. 1 contains a full description. In parallel, it was clear that MaX partners were interested in a stronger focus on the peculiarities of MAX - first and foremost, the exascale competency -, which are necessary to differentiate MAX offering from competing offerings that are appearing on the market. Taking into consideration these aspects (the importance of user interface to the code, and the importance of exascale), and some weaknesses of the QaaS that emerged in the meantime, the focus of the QaaS model was changed from a pay-per-use model to the development of a universal exploratory interface, based on the concept of the active notebook, that can be deployed on top of existing HPC infrastructures or in scientific cloud services (like the Amazon P3 GPU instances, or Azure HPC) to provide a simpler layer encapsulating the individual MAX codes and using the AiiDA platform as a universal data bus. The new QaaS interface was planned to be subject to the same consulting and software support services that are currently part of the MAX offering, with a business model similar to those widely used in open source software markets; in this sense, QaaS could be considered an additional open source code that can be offered by the HPC centres or that can be installed and integrated within a large company software chain, replacing the specific commercial offering based on pay-per-use. In practice, in the last years the QaaS model was explored and integrated in the services that are offered by MaX (via AiiDA lab, a cloud platform based on jupyter and jupyterhub AiiDA and most of the MAX flagship codes, and the use of Quantum Mobile— a VirtualBox machine that comes with AiiDA and a set of commonly used quantum codes preinstalled).

4.2 Definition of services

After surveying the opportunities and the potential match with the service activities that could be collectively offered by MAX members, the most relevant services were identified:

Service base	Description	Per-unit value	Potential scale
Knowledge	support, training on the scientific and technical aspects of quantum simulations	medium/ large	small/medium (experienced industrial and academic users)
Knowledge+code	support, training and code development related to the MAX software platform; optimization and porting; extending the platform, custom coding	medium/ large	small (large industrial and academic users)
Knowledge+code	integrating MAX codes with third-party codes and platforms, including proprietary ones; licensing and support for the open source aspects	medium/ large	small (software vendors)
Code+execution	"Quantum-as-a-Service": easy to use interface to MAX codes, delivered as a service or on-premise, helping to bring the world of HPC simulations to engineers and materials designers, enabling transfer of technology to commercial end-users	small	medium (academic and industrial users, including SMEs)

Table 2. Services that could be offered by MaX according to its business model.

The average contract size in Table 2 is estimated using data obtained from the current MAX partners concerning commercial services. In Ref. [1] the partners reported a set of consulting activities, mostly related to services like training, support and custom development, with per-year effort valued between 45K€ and 90K€ for custom development, and between 9K€ and 20K€ per year for support and training. These assumptions can be now updated to 2019 on the basis of a survey of commercial services performed by MAX partners. A summary is reported in Appendix 2, indicating major increases in the last year (up to 790K€ for code development and 265K€/year for services and training). As these are in part related to specific activities of some partner, we prefer a conservative approach and wait for the evolution and possible consolidation in the next year.

4.3 Value proposition for customers and for partners

The following main advantages that MAX can provide to customers are foreseen:

- Faster time to code custom features
- Faster know-how transfer through training with worldwide experts
- Access to pre-release code and algorithms
- Integration of bleeding-edge research into current simulation pipelines
- Simple implementation of simulation pipelines through private execution of code

It is essential for success as a sustainable entity that MAX can demonstrate that can provide services at a lower cost compared to what a company could do using internal resources; in this

sense, MAX commitment must be in demonstrating its excellence and capabilities to provide world-class research.

Concerning partners, MAX can provide them substantial value by helping in the commercialization and the continued funding of software development and improvement. MAX can provide value by:

- Financing software development: actively search of funding opportunities, coordination of application process, identifying potential commercial customers that may fund individual research activities
- Helping in the tendering and contracting process: MAX can provide legal support, licensing assistance, project management and coordination (for example in creating links between two separate software components); as well as facilitate the commercial contracting activity for entities that may have difficulties in accepting private contributions
- Reduction of time consuming tasks: helpdesk (one of the activities of greater success within MAX in terms of supporting software users) and dissemination activities to increase user attraction
- Code management and packaging: providing infrastructure and stable builds for users who expect stable and certified releases.

Expanding the customers' base will be an important component of activities. Among the ways to engage with potential customers, we focus on

- Direct prospect contacts
- Industry events
- Conferences
- Industry associations
- Website and online presence

Among these, direct contacts ("inside sales") have proven to be one of the most effective customer contact methods for MaX when focusing on mid- to large-size contracts, like consulting and training contacts; they require limited effort and expenses when compared with dedicated sales personnel, and have a comparable closing rate.

Additional channels are expected to develop within the European ecosystem, e.g. through collaborations with EuroHPC activities including the forthcoming HPC Competence Centers. Collaborations with such initiatives, in coordination with FocusCoE and other CoEs, may open new opportunities for user engagement, especially in industry.

4.4 Revenue and cost streams

In general, software business derive revenue in a number of different ways. A typical business model is based in most cases on a hybrid approach utilising a range of revenue models. In this

paragraph we first summarize the schemes identified in Ref. 2, and then describe the situation for MaX.

According to [2], revenue models relevant to materials modelling software in principle include the following: (a) Product Sales and maintenance services, (b) Subscription based software licensing, (c) Services and consulting, (d) Open-source based business models, (e) Government funding, (f) Software as a Service (SaaS), (g) Marketplace business models. MAX general strategy is centered on open source codes, which restricts the possible revenue models, essentially excluding (b) Subscription based software licensing. In Open-source based business models, (d), the main value comes from people with knowledge/expertise and this is their asset. The aim is to offer consultancy and solve customers' problems through code development and maintenance. Revenue is based not only on services, but also on OS-supported and ready-to-install versions, pre- and post-processing tools as well as materials relations (e.g. force fields) that work with the models encoded in open source software. It overlaps with (c) Services and consulting model, with services that range from very limited service of maintenance to more extensive implementation, customisation, training, technical support or consulting and contract research services. The revenue share generated by services cannot be standardized as it is somewhat related to product complexity as well as maturity of both the product and the market (i.e. user experience). Moreover services and consulting do not scale in the same way as software sale in terms of revenue and profitability (one can charge people per the hour/day only once, whereas software can be charged several times), and service engagements go through peaks and troughs, which can lead to resourcing issues. (f) Software as a Service (SaaS), a model that consists in providing the customers with the access to the software, is still in its infancy also among software companies, mainly due to security concerns by the industrial end-users. However, it could provide a faster route for new features to get to users and would help to reach small and medium enterprises, having the potential to attract customers that do not have the means to get infrastructure and skilled staff in place. For example, it could lead to getting into market niches, especially SMEs, that could not afford a code and the infrastructure needed. SaaS is also a good way to utilise substantial knowledge around a particular open-source software and to sell simulation services to experimentalists. It is thus worth to be considered as a possible future business model for MAX, although in the actual configuration we do not expect to be immediately feasible. Government and public funding models, (e), turn out to be essential in the case of development of new software or major upgrade operations: a materials modelling code can take 10 years (or more) of development to reach a level of maturity ready for industrial applications. In the business plan for MAX, the revenues will be calculated considering limited or no funding from public entities, as recommended in previous reviews of the CoE. However, this exercise will need to be re-analysed if the goal is to maintain the strong 'exascale-oriented character' of MAX, whose development critically rely on relevant public funding.

In the following we discuss a preliminary scheme for MAX, based on the main motivation and focus of its partners. We envision MAX as a legal entity capable of taking contracts related to materials modelling and simulation, and act as a project manager and legal facilitator, using resources from the MAX partners. Expenses are estimated in the hypothesis that MAX acts as a

lightweight support entity that mediates requests, performs project management and handles the technical infrastructure in addition to the software development and contract work. For a discussion of future legal structures to implement directly the support activities, see Section 5.

The new entity will focus and provide the following services:

- project and customer management (managing all aspects of procurement and interaction between the customer and the relevant research groups);
- software project management (handling third party developers that complement internal partners' development resources);
- bespoke software development;
- maintenance of the MAX platform infrastructure;
- dissemination and marketing to facilitate new business for the CoE.

Maintaining the assumptions about the analysis of the reference market (Section 3), the products and services achievable (Section 4) and the relationships among MAX Participants, which should aim at strengthening the collaboration, also through the commercial exploitation of the results, we gave mandate to an external consulting company to draft a three-year economic and financial plan [11] aimed at identifying the possible streams:

i. of revenues

ii. of reasonably reliable costs

basing on historical data available, re-modulated to take due account of the value of the resources (of personnel and instrumental facilities) that MAX Partners will make available both in cash and in kind. As the economic and financial plan is strictly related to the legal entity that MAX Partners will undertake, we first report a brief summary of the possible legal entity analysis in Section 5, and then present the financial plan in Section 6.

5. Analysis of legal instruments

The existing MAX CoE has been working as a mediator, an entity that provides support and project management to all the participating entities, and merely facilitates the take-up of services and contracts. While this role has been rather effective, some of the members have highlighted difficulties in taking up commercial activities due to the lack of current legal frameworks and difficulties in accounting services (prevalent especially in academic institutions). Difficulties are also envisioned in adopting resources for software development, especially when related to ancillary or support code where the high skills and knowledge of MAX experts are not strictly necessary.

We then gave mandate to an external consulting company for the exploration of potential structures that can help overcome these difficulties and, at the same time, can afford functions of coordination and consolidation of the MAX network and the development of further research

activities, as well as application, mainly commercial and therefore market-oriented, of knowledge and skills acquired after the MAX project and related updates.

In their report (Pinto and Sartore, Ref. [11]), three possible legal structures were analysed on the basis of the following parameters/requirements (which the chosen entity must be provided with):

A. Capacity and legal personality, liability: ability to be holder of rights and obligations, and liable for its obligations and its debts exclusively within the limits of its assets;
B. No-profit: from a thematic point of view the main purpose is the achievement of specific "ideal" objectives (research, development, etc.), and the commercial activities undertaken (oriented to the market) must be auxiliary and instrumental to it; from an economic point of view, possible margins and therefore possible profits cannot in any case be distributed to the participants / shareholders, since they must be retained and reinvested, for the pursuit of its main "ideal"purposes;
C. Suitability for business activities: the possibility to carry out market-oriented activities, with differentiated discipline according to its nature and purpose;
D. Relationships with participants, mutualistic purpose, transnationality: predisposition to use the competences of the Participants/ members (legally regulated on the basis of mutuality/consortium principles) and auxiliary nature of the activities carried out by the entity with respect to those of the members;
E. Access to national and EU financing: the possibility to access the various financing measures, deriving from public contribution or linked to national and EU funds;
F. Social capital: the obligation to provide the entity with an own endowment capital fund, generally expressed in cash;
G. Other aspects: employee recruitment and main fiscal aspects.

On the basis of these considerations, three entities were considered potentially suitable for the purpose. In Ref [11] it was assumed for convenience that the "Legal Entity" may have its registered office in Italy; therefore the requirements described above were analysed with respect to specific forms of "Legal Entity" existing in the Italian legal system. However, these are not extraneous to other Community Regulations and may serve as a guideline for the discussion among partners. The extension of the analysis to cases of regulations different from the Italian one may be developed later on.

The three types of "Legal Entity" identified in [11] are the following:

1. the European Economic Interest Grouping (E.E.I.G.), an institution of EU origin [12] that, in the context of the single market, responds to the need "to facilitate or develop the economic activities of its members and to improve or increase the results of those activities";
2. the Consortium Company with limited liability (SCaRL), an Italian civil law institution, that can be defined as a joint capital company which, instead of pursuing a lucrative purpose, pursues consortium-mutualistic purposes;
3. the recognized Association, an Italian civil law institution, which is reserved for legal entities other than the Companies, but it is provided also by the legal systems of the

majority of the EU countries; it is aimed to fulfill aggregation needs felt by individuals or legal entities, both public and private and it is established for the pursuit of "ideal" no-profit scopes.

The following two tables summarise the parameters/requirements of each legal option, their analysis in terms of strengths and weaknesses and main conclusions:

Legal Entity / Requirements	1. European Economic Interest Grouping (E.E.I.G.)	2. Consortium Company with limited liability (SCaRL)	3. Recognized Association
A. Capacity and legal personality	NO legal personality and the members ARE liable for the grouping's debts , without any limitation.	It has legal personality and its Shareholders ARE NOT liable for the Company's obligations and debts, except within the limits of the capital contributed.	It has legal personality and the Members ARE NOT liable for the Company's obligations and debts, except within the limits of the associative fund conferred.
B. No-profit	The absence of a profit is overcome by its auxiliary function	The absence of profit is coherent to the mutualistic purpose. It is allowed, making use of the resources of the Members and coordinating them, to approach the market applying prices compatible with the market rules, thus creating margins and making profits, which must be set aside and cannot be distributed to the Members.	The absence of profit is consistent with the nature of the Association, thus assuming the legal prohibition of distributing profits to Members, even if the allowed ancillary economic activity can make margins and profits, which must be set aside.
C. Suitability for business activities	It typically carries out business activity. It must be registered to the Italian Commercial Register with commercial companies' requirements (accounting records, balance sheet filing, appointment of directors).	SCaRL, as established as a company, exercises business activity as a presumption. It must be registered to the Italian Commercial Register with commercial companies' requirements (accounting records, balance sheet filing, appointment of directors).	The Association, as constituted for the pursuit of "ideal" purposes, does not have as its main activity commercial activity in the form of a business company; it can carry out an economic activity, ancillary to the main activity, with gaining of financial resources to support the main “ideal” activity.
D. Relationships with participants	It routinely uses the services, skills and facilities of its Members. It requires the participation of at least two Members from two different EU States and prohibits participation of non-EU Members States. Profits and losses are distributed among the Members according to the Group contract or in equal parts.	The mutual-consortium purpose is coherent to the legal nature of the consortium company. This tool appears to be the ideal one in the case of public entities that intend to create an initiative dedicated to the performance of economic activities. The requirement of transnationality, in terms of relationships with the EU, does not appear to be directly satisfied. Members from non-EU Member States are allowed.	The relationships among Association and the Members, if they have economic-commercial contents, are "attracted" to the business activity regime for both parties, and as such they are also regulated for fiscal purposes both by the Association and by the Associates. The requirement of transnationality, in terms of relationship with the EU, does not appear to be directly satisfied. Members from non-EU Member States are allowed.

E. Access to national and EU financing	It has access to EU funding and meets with the requirement of transnationality on the assumption that the activities are carried out by the Participants, who act as natural "linked third parties". The ownership of the results may move from E.E.I.G. to one or some of its Members. Its profile can be Private body / SME or Research Organization.	For a SCaRL, access to EU funds appears configurable within the Private body / SME. Moreover, taking into account the constraints of non-distribution of profits, it seems reasonable to verify the possibility of framing the SCaRL alternatively as Non-profit Organization.	The access to EU funding appears to be configurable within the Non-Profit Organization. the Association/Members relationship complies with the requirements to be able to define the Members as "linked third parties", thereby allowing the Association access as "sole beneficiary".
F. Social capital	The payment of a minimum endowment fund is not required.	For the establishment of a SCaRL, the Italian civil code imposes a capital amount not less than 10,000.00 euros.	For the recognition of legal personality to the Association it must be established a patrimony adequate to achieving its purposes. According to a consolidated practice, in Italy it is considered as adequate a conferred assets not less than € 75,000 / 100,000. For the determination of the initial Endowment Fund it is not possible to overlook the results of the Economic-Financial Plan, with particular regard to the cash flow analysis and the capital endowment considered sufficient to guarantee financial balance.
E. Other aspects	It can be an employer (limited to 500 persons). Italian general laws on employment relationships for companies. E.E.I.G. is a VAT payable subject and therefore subjected to all related accounting and tax obligations. It is not subject to other direct taxes (IRES - IRAP).	The SCaRL can be an employer, without any limitations, except in compliance with the current legislation. Italian general laws on employment relationships for companies. The participation by Public Bodies in commercial companies presents, in principle, some critical points, which require further study, including comparative international law.	The recognized Association can be an employer, without any limitation, except the respect of the current legislation. Concerning the fiscal regime of the "Association" option, the analysis of the Economic-Financial Plan will be decisive: the prevalence of economic activities (even auxiliary) with respect to “ideal” activities involves the fiscal attraction of all the activities carried out by the Association under the corporate income regime, both for VAT purposes and for direct taxes. Participation by Public Administrations in Associations is not, in principle, subject to particular constraints/limitations, except compliance with the procedures and authorizations required by the system of governance of each

			adherent Entity.

Table 3. Legal entity comparison chart [11].

	Strengths	Weaknesses	Conclusion
Legal Entity			
European Economic Interest Grouping (E.E.I.G.)	a) The E.E.I.G. it is the natural aggregation tool for subjects belonging to different countries Member of the European Union; b) The E.E.I.G. it is an ideal tool for carrying out economic activities, not excluding however the possibility of carrying out research and development activities, even financed, having essentially regard to community financing, on which the requirement of transnationality is automatically achieved; c) By legal nature, the E.E.I.G. is established in order to involve its members in the activity.	a) The E.E.I.G. is characterized by a regime of unlimited joint and several liability of the Members for the obligations contracted by E.E.I.G.; b) the losses of E.E.I.G. are attributed to each Member in proportion to the participation resulting from the contract or, failing that, in equal parts; c) the fiscal regime for the taxation of income earned by the E.E.I.G. presents elements of complexity, especially for non-residents, above all for Members who have the nature of a Public Body, both resident and non-resident.	Weaknesses are critical enough to make the E.E.I.G. as not advisable option
Consortium Company with limited liability (SCaRL)	a) The SCaRL is the natural aggregation tool of Entities that intend to carry out business activities in pursuit of non-profit-making but gaining economic advantages for the consortium members, in a mutualistic key; b) Consortium members can also belong to countries that are not members of the European Union; c) The SCaRL has legal personality, and is responsible for its obligations and debts exclusively within the limits of its assets, without the shareholders involvement; therefore, Members are NOT subject to the regime of unlimited joint and several liability for the obligations contracted by ScaRL, and limit their risk to the amount of the contributions due and made; d) From a fiscal point of view, the SCaRL is an independent tax Entity. e) From a legal point of view, the SCaRL is typically the subject of coordination and synthesis of the competences and resources made available by its own Consortium members.	a) The attraction to the business regime of all the activities carried out leads to believe that every activity of the SCaRL must be finalized to the realization of a business activity; this approach can lead to disadvantages (of a fiscal nature) for activities that may be carried out that are not immediately attributable to economic activities (we refer, typically, to self-financed research activities). b) Having acknowledged that the main purpose of a commercial company, even if it is a consortium, is in any case the carrying out of economic activities, the possible support to activities characterized by merely ideal purposes (research and development not linked to the production of revenues), could create legal difficulties, which must also be considered in terms of possible internal governance conflicts for the participating public bodies	The strengths and weaknesses present an overall framework characterized by a substantial balance.

Recognized Association	a) The "recognized Association" is the natural aggregation tool of Subjects who intend simultaneously to pursue "ideal" goals and objectives (research, development, etc.); set up a non-profit entity, able to pursue mutualistic purposes, set up an entity who can also carry out economic/commercial ancillary and instrumental activities, with respect to "primary" activities, identifiable in their "ideal" goals. b) The "recognized Association" has legal personality, and is responsible for its own obligations and debts only within the limits of its assets, without the Members being subject to the regime of unlimited joint and several liability for the obligations contracted by the Association; c) From a fiscal point of view, it is an independent tax subject; d) Members may also belong to countries that are not members of the European Union. e) Concerning transnationality and access to EU funds, the Associative instrument, as it is participated by Entities belonging to different Member States, appears to be potentially implementing the requirement of transnationality, and it is certainly admitted as Entity entitled to coordinate the activities of its participants such as "linked third parties" of the beneficiary association.	Given that the primary purpose of the Association is to carry out research and development activities, the prevalence of commercial activity over institutional activity does not conflict with the choice of the "Association" option if this prevalence, only quantitative, does not diminish its character of "ancillarity" to the primary ("ideal") activity. Conversely, if the facts were to prove that the main purpose is the economic exploitation of the knowledge and commercial impact of results of the MAX project, leaving research and development as secondary, the "Recognized Association" option would prove to be unsuitable for the purpose.	Since the strengths appear to be of the utmost importance, while the weakness can be overcome once the actual association aims are confirmed, the "recognized Association" option appears to be evaluated favorably.

Table 4. Legal entity SWOT analysis [11].

As illustrated in the tables, a preliminary conclusion is that the "recognized Association" option appears to be the most favorably evaluated as Legal Entity for MAX.

The economic and financial analysis relating to the three-year development of the activities of the above identified Legal Entity are illustrated in the following section.

6. Economic and financial plan

This section reports the economic and financial analysis, relating to the three-year development of the activities of the above identified Legal Entity, as performed by A. Pinto and C. Sartore in their study (Ref. 11).

The business plan was drawn up on an annual basis and then developed over a three-year period: it was not considered appropriate to develop a business plan for a longer period, as the data would not be characterized by an appreciable degree of reliability. The costs and revenues included in each annual plan have been estimated on the simplifying assumption that each year spans from 1/1 until 31/12. If the first year was of shorter duration, the data had to be reduced appropriately in application of a principle pro rata temporis.

The plan contains working assumptions related to the characteristics of a recognized Association, since option 3 was preliminarily evaluated to be the most appropriate for the MAX case (see Section 5).

In addition, it is based on the historical data recently collected by the MAX Partners, concerning the description and valorisation of the activities carried out by each of them towards customers in responding to their service needs.

Two criteria of classification of the economic elements have been used to draw up the plan, corresponding to their "nature" and "destination". Revenues and costs have been accordingly detailed as follows:

Criterion	**Revenues**	**Costs**
A. by "nature"	❑ Consulting ❑ Code Development ❑ Training ❑ Other activities	❑ Management activities ❑ Marketing activities ❑ Operation/ general expenses
B. by "destination"	❑ Revenues from provision of services ❑ Contributions for projects financed externally by the EU or other national / international public bodies ❑ Membership fees ❑ Contributions in –kind for resources made available by Members.	❑ Personnel costs (researchers, technicians, administrative) ❑ Costs for technical-scientific services provided by Members ❑ Costs related to funded activities ❑ Costs related to internal projects (funded by Members with membership fees) ❑ Costs related to resources attributed in kind by the Members ❑ Costs for services provided by third parties ❑ Amortization/depreciation ❑ Other general expenses ❑ Financial charges ❑ Taxes.

Table 5. Criteria of classification of economic elements.

It is estimated that in the three-year period there will be no need for investments in additional own assets: possible needs for such investments can only be speculated starting from the third year, when it will be necessary to have full knowledge of the economic/financial self-sustainability of the proposed initiative.

Note that the contributions from the EU and other public bodies are included here at a marginal level, with minor revenues corresponding to typical small funding for startup projects. This exercise largely underestimates what we expect from national / international projects (beyond the CoE direct funding) on the basis of the relevant contributions obtained by MaX partners from these sources in the last years.

	REVENUE CENTERS				COST CENTERS			
YEAR "N"	Consulting services	Code development	Training	Others	Management	Marketing	General expenses - operation	**TOTAL**
Revenues from provision of services	100 (a)	200 (a)	10 (a)					310
Contributions (funded activities)		50 (c)						50
Membership fees				30 (d)				30
In-kind contributions					18 (e)	9 (e)	21 (e)	48
(A) Total value of production								***438***
Personnel costs							9 (f)	9
Services costs provided by Members	65 (b)	150 (b)	7 (b)					222
Costs related to funded activities		40 (c)						40
Costs related to internal projects				30 (d)				30
Costs related to in-kind contributions					18 (e)	9 (e)	21 (e)	48
Services costs from suppliers	5 (g)	10 (g)	1 (g)			20 (g)	12 (g)	48
Amortisation, depreciation								
Other costs							13 (h)	13
(B) Total costs of production								***410***
(C) Financial expenses								0
(D) = (A) - (B) - (C) Result before taxes								***28***
(E) Taxes on the income for the year								8
(F) = (D) - (E) Net profit (loss) for the year								***20***

	REVENUE CENTERS				COST CENTERS			
YEAR "N+1"	Consulting services	Code development	Training	Others	Management	Marketing	General expenses - operation	**TOTAL**
Revenues from provision of services	110 (a)	220 (a)	11 (a)					341
Contributions (funded activities)		63 (c)						63
Membership fees				30 (d)				30
In-kind contributions					27 (e)	18 (e)	18 (e)	63
(A) Total value of production								***497***
Personnel costs							18 (f)	18
Services costs provided by Members	72 (b)	165 (b)	8 (b)					244
Costs related to funded activities		50 (c)						50
Costs related to internal projects				30 (d)				30
Costs related to in-kind contributions					27 (e)	18 (e)	18 (e)	63
Services costs from suppliers	6 (g)	11 (g)	1 (g)			5 (g)	15 (g)	37
Amortisation, depreciation								
Other costs							15 (h)	15
(B) Total costs of production								***457***
(C) Financial expenses								0
(D) = (A) - (B) - (C) Result before taxes								***40***
(E) Taxes on the income for the year								12
(F) = (D) - (E) Net profit (loss) for the year								***28***

	REVENUE CENTERS				COST CENTERS			
YEAR "N+2"	Consulting services	Code development	Training	Others	Management	Marketing	General expenses - operation	**TOTAL**
Revenues from provision of services	127 (a)	253 (a)	13 (a)					392
Contributions (funded activities)		75 (c)						75
Membership fees				30 (d)				30
In-kind contributions					18 (e)	18 (e)	18 (e)	54
(A) Total value of production								***551***
Personnel costs					9 (f)		18 (f)	27
Services costs provided by Members	82 (b)	190 (b)	9 (b)					281
Costs related to funded activities		60 (c)						60

Costs related to internal projects				30 (d)				30
Costs related to in-kind contributions					18 (e)	18 (e)	18 (e)	54
Services costs from suppliers	6 (g)	13 (g)	1 (g)			5 (g)	15 (g)	40
Amortisation, depreciation								
Other costs							16 (h)	16
(B) Total costs of production								***508***
(C) Financial expenses								0
(D) = (A) - (B) - (C) Result before taxes								***43***
(E) Taxes on the income for the year								13
(F) = (D) - (E) Net profit (loss) for the year								***30***

Table 4. Business Plan.

KEY:

(a) Revenues from the provision of services (Consulting, Code development and Training) of year "N" have been estimated on the basis of the average value of the services already provided in the past by some of the MAX Participants, while for years "N+1" and "N+2" on the assumption of improvement prudentially estimated at 10% and 15% respectively.

(b) Costs directly related to the production of the services have been estimated for all the three years on the basis of the average value of the direct production costs of the services provided (by the Members), calculated by applying the percentage obtained by the same historical data: 65% for Consulting, 75% for Code development and 70% for Training. The contribution margin for services is therefore supposed to be around 30% on average.

(c) It has been assumed that the Legal Entity can apply for public funding projects (national/international): the direct costs have been estimated with a view to applying a flat rate to cover the overhead, according to H2020 calculation rules (100% financing and 25% overhead). Compared to the year "N", the amount of contributions on funded projects has been slightly progressively increased over the years "N+1" and "N+2".

(d) In order to support, during the initial phase, the start-up of internal projects of a scientific-technological nature, revenues deriving from Membership fees have been assumed entirely to cover the costs of these projects and unchanged for all three years.

(e) Contributions "in-kind" by Members in the 3 years are assumed as follows:

	Year “N”	Year “N+1”	Year “N+1”
personnel	3 units of staff: -1 secretarial 50% for 6 months (estimate 9k€); -1 technical-scientific management	2 units of staff: -1 technical-scientific management coordination area 30% (estimated cost 27 k€);	2 units of staff: -1 technical-scientific management coordination area 20% (estimated cost 18 k€);

	coordination area 20% (estimated cost 18 k€); -1 marketing area 10% (estimated cost 9k€)	-1 marketing area 20% (estimated cost 18k€)	-1 marketing area 20% (estimated cost 18k€)
utilities by location and operating services	12k€	18k€	18k€

(f) It has been assumed that starting from the second half of the year "N" the conditions are met for the direct hiring of a person (part time 50%) in charge of the general operation and secretariat of the Association, estimating an annual cost of 18k€. At years "N+2" it is assumed to hire 1 further employee on secondment from a Member with coordination/management functions (10% of the annual cost of 90k€).

(g) It has been assumed that the Association shall purchase services from third parties, both with reference to activities of Marketing (equal for year "N+1" and "N+2", but less than the year "N") and Operation (equal for year "N+1" and "N+2", but slight more than the year "N") , and with reference to the services acquired by the Members (see note b.).

(h) In the "other costs" item, general costs and "contingencies" have been estimated around 3% of the production value for all three years.

Besides the economic plan, a detailed cash flow statement over the three-year period has been prepared in order to verify both the financial sustainability of the plan and the measurement of cash requirements: in this regard, it should be noted that the initial Endowment Fund is considered sufficient with respect to the need to cover the initial cash requirement if it will be fixed in an amount of 100K€.

7 Conclusions

This work has analyzed the potential market, the business model (value proposition, services, revenue and cost streams), the legal instruments and the three-year economic and financial plan in order to assess the possibility to set up MaX as a self-sustainable legal entity essentially based on commercial activities. Public funding deriving from national and international institutions and projects was intentionally included only at a marginal level at this stage.

The main conclusion is that a MaX entity essentially based on commercial activities would be sustainable beyond the end of the current H2020 funding period. This entity would carry out a large set of consulting and service activities of great relevance to the European HPC ecosystem and economy, but would probably be unable to sustain the research activities aimed at extreme

computing and frontier innovation which are currently at the core of MaX, as they require long term investments beyond what could be sustained by commercial activities alone.

Further details, and the interest and role of the different MaX partners in this initiative, will have to be assessed in the next one to two years.

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Appendix 1 - Industrial uptake.

The following companies have had a contact with MAX members for collaboration and commercial purposes.

Air Liquide	https://www.airliquide.com/	France
AMD	https://www.amd.com/en	USA
ANSYS	https://www.ansys.com/	France
ATOS	https://atos.net/en	France
BI-REX	http://bi-rex.it/	Italy
Comsol	https://www.comsol.com/	USA
Dassault Systèmes SIMULIA	https://www.3ds.com/products-services/simulia/?wockw=SIMULIA	USA
DYNAmore GmbH	https://www.dynamore.de/en	Germany
Exabyte.io	https://www.exabyte.io/	USA
Goldbeck Consulting	https://materialsmodelling.com/	UK
Hexcel Composites Ltd.	https://www.hexcel.com/	USA
Johnson Matthey	https://matthey.com/	UK
Moxoff	https://www.moxoff.com/	Italy
Nokia	https://www.nokia.com/	Finland
NVIDIA	https://www.nvidia.com/en-us/	USA
QWED	https://www.qwed.com.pl/	Poland
RED Fluid Dynamics	http://www.red-fluid.com/	Italy
Repsol	https://www.repsol.com/en/index.cshtml	Spain
Saipem	https://www.saipem.com/en	Italy
SINTEF	https://www.sintef.no/en/	Norway
Software for Chemistry & Materials	https://www.scm.com/about-us/	Netherlands
Synopsys Denmark ApS	https://www.synopsys.com/	Denmark
Tetra Pak Packaging Solutions	https://www.tetrapak.com/	Sweden
Toyota Central R & D Labs	https://www.tytlabs.com/	Japan

Appendix 2 - List of commercial contracts by MaX partners in 2018-2019.

Source	Year	Type of service	Short description of the activity/service provided	Customer business area	Duration of activity/ service (months)	Revenue (K€)
BSC	2018-2019	Consulting	Consulting about atomistic simulations	Manufacturer (end user)	12	120
BSC	2018-2021	Code development	Code optimization	Hardware manufacturer	36	330
CINECA	2019	Consulting	car-parrinello simulation setup, test and optimization of a small protein in water	Manufacturer (end user)	4	10
CINECA		Consulting	car-parrinello simulation setup, test and optimization	Manufacturer (end user)	2	5
EPFL	2019	Materials discovery	New solid-state electrolytes	Chemical Industry	24	ND
EPFL	2019	Materials characterization	Ferroelectrics	Electronic industry	24	ND
EPFL	2015	Materials discovery	Metal alloys	Watch industry	48	ND
EPFL	2020	Materials discovery	Qubits	ICT		ND
ICN2	2018-2019	Consulting	Atomic modeling of oxygen mobility in materials for oxygen sensors	Manufacturer (end user)	24	ND
ICN2	2019-2021	Consulting & training	Consulting about the use of SIESTA for the study of topological insulators	ISV		70
CNR	2019	Training + Support	Training; support concerning QE+QM/MM	Manufacturer (end user)	12	25
CNR		Code development	Consulting/code development	Hardware company	18	17
E4?	2017	Consulting	porting and optimizazion of codes	Manufacturer (end user)	6	30
SISSA	2018-2019	Code development	Software on demand	Software developer vendor	24	110
SISSA	2013-2018	Code development	Study of materials modelling	Food company	60	130