D10.4

Final Business Plan: exploitation and sustainability; uptake

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D10.4 Final Business Plan: exploitation and sustainability; uptake

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Version	Date	Author	Notes
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Executive Summary

This report updates the preliminary business plan and discusses the sustainability of the activities of the MAX European Centre of Excellence beyond the current H2020 funding scheme.
The first part resumes and updates 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 refreshed 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 interest and role of the different MAX partners in setting up a legal entity have been discussed in the last two years also in the framework of collaboration of CoEs within the FocusCoE CSA. 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, 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 far beyond what could be sustained by such entity.

1. Introduction

MAX is a European Centre of Excellence for High Performance Computing (HPC) focused on the domain of materials simulation, modelling and design. Its mission centres 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 beginning of its second phase (2019-2022), MAX presented a report where a general exploitation strategy of MAX results was analyzed with special reference to the potential market size and the individual value components [1].
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 same report presented an update and extension of this 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 that 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, was presented to assess this hypothesis.

2. 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 deliverable D10.2 Draft business plan: preliminary exploitation strategy. It is updated taking into account a more recent study by Goldbeck et al. [2].

Based on the data collected about the activities of the MAX CoE as a whole and of MAX partners, as well as the current literature, the "users" of the current MAX codes have been broadly classified 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.

2.1 Industry

MAX users in industry include:

- Commercial developers or vendors of materials simulation software (often named independent software vendors, ISV)
- Manufacturers (end users): This group represents the end-users of materials modelling in the 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.
- Translators [3], companies which are bridging from software owners or vendors to end users. Starting from an industrial problem, they identify a workflow for its solution by using materials modelling, acting as consultants for large manufacturers in the Materials Design process. Their activity faces the identification of all quality attributes within the language of the context of the technical industrial problem. This includes non-technical cost measures, such as the influence of the solution on the final pricing, and time to market. In the category some vertical groups are also included, like engineering specialists that "package" simulation workflows in custom software systems [6]. While the underlying simulation code is open source, the packaging provides an easy-to-use interface that automates most parameter building and post-processing.

An additional category of interest is that of HPC hardware companies. While they are not proper users of MaX, they do express interest and support for applications and for MaX initiatives enabling their best use and performance.

The amount of data on the size of the market for quantum materials simulation software is still very limited, in part owing to the very small size of the market itself that limits the interest of consulting companies in performing such measurements. The only analysis with a clear methodology is from Goldbeck Consulting in its first report from 2012 [7].

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 [7] 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, [8] 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 modelling 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 [5,9] 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.

To further validate the market size estimate in industry, we performed an analysis of the job postings in the Psi-K job list, the bottom-up researchers' network to build strength and cooperation in the field of computational electronic structure, the average 50% of positions are for post-doc or research assistants. Of these, less than 10% are requested from outside academia, mainly private research centres or software companies looking for personnel, e.g. BIOVIA, SUPCON Technology Co., and others. 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 [11] 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.

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). Analysing the market shows that adoption is concentrated on one very large vendor (Biovia/Accelrys) plus 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.

Analysis of the materials modelling market reported in the draft business plan ("D10.2 Draft business plan: preliminary exploitation strategy", M12) is still substantially valid in terms of field of applications of materials modelling software and market segmentation.

In September 2020, a new market research report on materials modelling software was published by Goldbeck et al. [2], where a focus on the study of materials in any field by any type of physics-based model was provided. The total market size for materials modelling software is here estimated to be in the range of €339.5m, based on an analysis including the major companies active in the field as well as a relatively large number of small companies (total of 72). The share of discrete (electronic/atomistic/mesoscopic) modelling is in the range of €85m, i.e., about 25% of the materials modelling market, against 75% due to continuum modelling.

As the focus of the big enterprises is more on engineering modelling, the materials modelling market is dominated by a large number of small enterprises (up to 50 employees) making up about 76.4% of the players, and most business is located in the €1m to €5m range, for both discrete and continuum modelling.

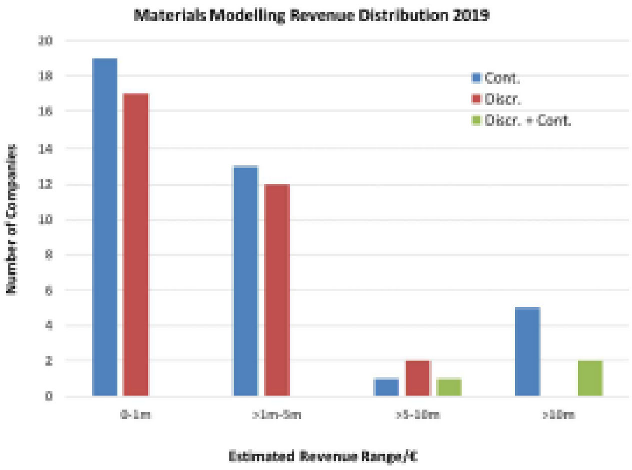

Fig. 1. Materials modelling revenue distribution for providers of continuum and discrete modelling software. (Source Goldbeck et al. [2])

About 80% of all considered companies showed an estimated revenue of up to €5m related to materials modelling. The pure discrete materials modelling software market is distributed across a wide range of players mostly up to €5m revenue with only 6% in the €5-10m bracket. Typically, these are pure discrete modelling providers. The picture is very different for the continuum modelling market, where providers feature in all revenue brackets. The discrete and continuum markets are still largely served by distinct players rather than integrated providers, and all providers of both materials modelling types are large enterprises.

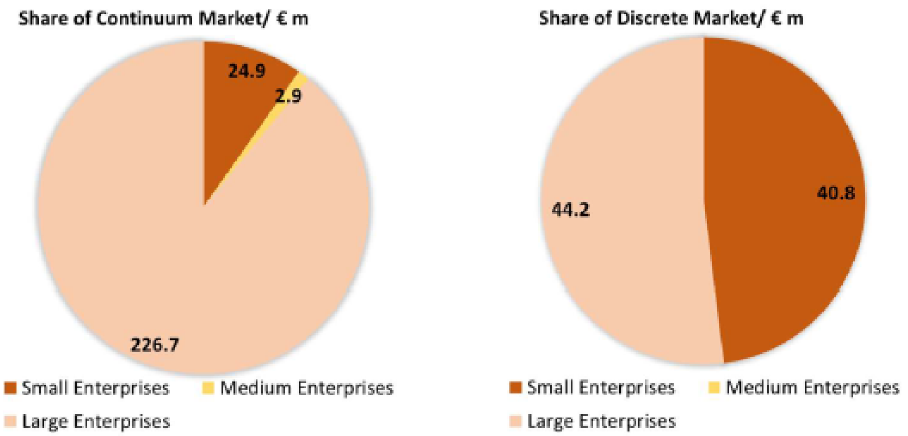

Fig. 2. Market shares for the continuum and discrete market (Source Goldbeck et al. [2])

The discrete modelling market is served by a wider range of providers in terms of size with nearly half of the market still captured by SMEs, while 89% of the continuum modelling market is served by large enterprises due to the very large size and wide use of their continuum modelling packages.

In addition to the commercial software market, there is what could be called a “hidden” market served by free and open source software (FOSS). In order to estimate a monetary value (which by no means can provide a full estimate of economic value) Goldbeck et al. [2] look into the amount of investment required to cover staff costs including overheads. Budgets to cover these are mostly provided by grant bodies in the case of FOSS. To keep things straightforward, they took the same amount of € 150k per FTE as in the company revenue estimates. Numbers of staff were typically based on the number of developers of the codes which can be obtained from websites and/or activity on public repositories such as GitHub. Since FOSS software is often limited to highly-skilled users, industrial use may require substantial additional investment in expertise and training which is not included in their estimates.

As it appears in the table below (Source Goldbeck et al. [2]), the total FOSS market contributes €29.3m.

Type of modelling	**Estimated investment**
Electronic FOSS software	€14.9m
Atomistic FOSS software	€6.9m
Mesoscopic FOSS software	€4m
Continuum FOSS software	€3.6m

Table 1. Electronic FOSS software market value (Source Goldbeck et al. [2])

The FOSS electronic modelling market considered by Goldbeck et al. [2] is composed of the software listed in the following table (where the ones used by MAX are evidenced in bold characters) and these codes are supported by an estimated investment of €14.9m.

Code	**License**	**Info**
AbInit	GPL	https://www.abinit.org/
CASTEP	Proprietary Academic free and commercials are charged	http://www.castep.org/Main/HomePage
CONQUEST	MIT	http://www.order-n.org/
CP2K	**GPL**	**https://www.cp2k.org/**

DALTON	LGPL v2	https://daltonprogram.org/
deMon2k	Proprietary Academic free and commercials are charged	http://www.demonsoftware.com/public_html/index.html
Fleur	**MIT**	**http://www.flapw.de/MaX-4.0/**
NEMO-3D	LGPL v2	https://engineering.purdue.edu/gekcogrp/softwareprojects/nemo3D/
NWChem	Educational Community License 2.0 like Apache	https://nwchemgit.github.io/
OpenMX	GPL v3	http://www.openmx-square.org/
QuantumEspresso	**GPL**	**https://www.quantum-espresso.org/**
Siesta	**GPL**	**https://departments.icmab.es/leem/siesta/**
The Elk Code	GPL	http://elk.sourceforge.net/
Yambo	**GPL**	**http://www.yambo-code.org/**

Table 2. SW considered in Electronic FOSS software and its licensing (Source Goldbeck et al. [2])

Tentative figures for market dynamics, reported in the work by Goldbeck et al. [2], indicate a long term growth in the discrete modelling market of about 5% in contrast to a roughly 10% pa growth in continuum modelling. They conclude by arguing that there are likely to be substantial changes ahead due to further integration of materials into CAE combined with a strong growth in data-based, machine-learning methods for materials. They expect to see a confluence of materials modelling and data technologies into a broader materials informatics market, where physics-based models together with experiments provide a source of data as well as insights, while data-based models, ML and AI greatly enhance the capability to utilise heterogeneous knowledge sources for maximum benefit. Finally, there is a nascent market in quantum-computing solutions for computational chemistry. There is growing interest in this potential breakthrough technology, with chemistry and materials science covered by some large enterprises with hardware interests (e.g. IBM, Google) as well as dedicated quantum computing software providers and SaaS providers.

2.2 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 user 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: though we reckon we cannot give complete figures, we can assess the broadness of our flagship codes' users by looking at interactions they had in these years. An example is given in the table below (from D7.3 Third (final) report on the activity of the High-Level Support services (third year), M46) that summarizes the support operated by MAX personnel and by the code communities in M24-46. Analysis of data shows that the greatest number of users are academic and governmental researchers. Moreover, around 1,500 people attended MAX schools and hackathons, being (interested) code users, and almost all of them were from academia, for a total of 22 (co)organized events.

MAX Codes	Number of incoming threads	Total number of emails/posts	Gitlab threads	Number of face-to-face support activities	Number of slack messages
QE	434	610	102	8	1367
Siesta	212	573	89	12	-
Yambo	504	1054	-	26	-
BigDFT	-	-	17	6	40400
Fleur	153	627	243	1	-
AiiDA	110	410	851	11	53797
Total	1413	3274	1302	64	84314

Table 3. Numbers of contacts operated by MAX services (from D7.3, M46)

- Citations: the number of publications explicitly citing the use of four MAX codes (QuantumESPRESSO, SIESTA, CP2K, Yambo) sums up to 4302 in 2021. The average overall growth rate moved from 9.5% in 2019 to 15%, clearly mirroring the increasing interest in atomistic codes. The data have been collected from the website https://atomistic.software/#/ by Leonard Talirz, EPFL (doi 10.5281/zenodo.4639414) [10].

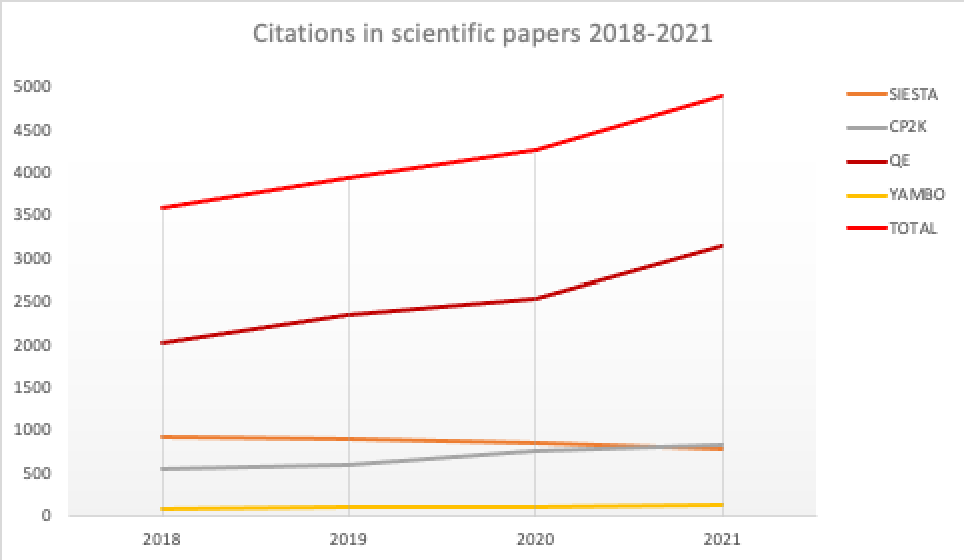

Fig.3. A chart showing the growth of flagship codes citations growth in 2018-2021 (Source: https://atomistic.software/#/)

3. Business model

3.1 Identification of value components

The components that form a business model are (1) value architecture (revolving around organisational resources and capabilities as well as their configurations); (2) value network (representing the external arrangements which revolve around the communication and collaboration that the organisation 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 (3) value finance (revolving around the financial arrangements the business organisation 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 in order to 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 current service activities of MAX as listed in Table 4. The table has been edited with respect to the one in D10.x in order to better describe the MAX activities.

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 (parallel) configuration in order to obtain the best performance in calculations; ° ad-hoc solutions for users, possibly including custom code development; ° dedicated consulting and support for the development of new features in MAX codes	WP1 to WP7	x x x	x x x	x x x	x x x
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 Tier0 HPC machines.	WP5, WP7	x	x x	x x x	x x
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	x x	x x x	x x
4. Training	° workshops and schools on HPC applications in materials sciences ° contributions to University courses (undergrad and graduate level) ° training through research in MAX labs ° specific training activities for industrial end-users	WP8	x x x	x x x	x x x	x x x

5. Container technology for HPC systems	° exploiting container technologies for MAX codes on HPC systems (docker, shifter, singularity)	WP5, WP7	x x	x x	x x x	x x x
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	X x x	x x	x	x x x
		**number of x indicates relative uptake (past and current) by different target users*				

Table 4. Services offered by the MAX CoE.

Knowledge.

- Specific training activities for industrial end-users;
- training through research in the CoE labs;
- contributions to 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 (parallel) configuration to run calculations in order to obtain the best performances;
- ad-hoc solutions for users, possibly including 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.

Code.

For code, the relevant value proposition is mediated by the licensing, that for all MAX codes is open source. 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 licence 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 licence. Since the MAX codes are under an open source licence, this integration raises some additional difficulties related to licence compatibility and in general licence compliance; this model has led to the signature of a substantial contract with the US commercial software developer Schrödinger[1], that requested support for integrating one of MAX codes (Quantum ESPRESSO) within their modelling and simulation suite. Similar exploitation is done by SIMUNE Atomistics SL[2], a spin-off company founded by some of the original developers of SIESTA, that has built a business model for developing software products and tools around SIESTA.

Other combinations may not be considered profitable for MAX, such as **Execution** and **Knowledge+Execution**, for they are more of interest to HPC providers and show no added value from MAX capabilities and codes. Similarly, **Knowledge+code+execution** would mean to consider MAX as a single-stop-shop where the end user would be able to get training, support, and also execution of workloads. It would be equivalent to the superposition of already described models, with no additional value added.

[1] https://www.schrodinger.com/products/quantum-espresso
[2] https://www.simuneatomistics.com/

Code+Execution.

This combination can be considered equivalent to the general concept of SaaS (Software as a Service). A possible model, named QaaS (Quantum-as-a-Service), was 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.

Taking into consideration the importance of user interface to the code, 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).

3.2 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 5. MAX Services that could be offered according to its business model.

The average contract size in Table 5 is estimated using data obtained from the current MAX partners concerning commercial services. In D10.2 a list of consulting activities performed by partners was given (Appendix 2). It indicated a major increase in 2019 revenues (up to 790K€ for code development and 265K€/year for services and training). An updated list is given in this deliverable, updated to 2022, that instead shows a very reduced commercial activities by partners.

3.3 Value proposition for customers and for partners

To be competitive as a (paid) service provider for customers, MAX identified a few features that should necessarily be ensured, such as:

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

Moreover, it is essential for the success as a sustainable entity that MAX can provide services at a cost that is lower than what a company would spend using internal resources; in this sense, MAX commitment must be in demonstrating its excellence and capabilities to provide world-class research.

To partners MAX can provide substantial value by helping in the commercialization and in supporting and financing the software development and improvement. MAX thus 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.

Exploitation and uptake actions aimed at expanding the customers' base are an important component of activities. Among the ways to engage with potential customers, we focus on (i) direct prospect contacts; (ii) Industry events; (iii) Conferences; (iv) Industry associations; (v) 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 Centres. Collaborations with such initiatives, in coordination with FocusCoE and other CoEs, may open new opportunities for user engagement, especially in industry.

As an example of the expertise in this field, we point out that MAX has already developed and attended a series of dissemination actions, such as 36th International CAE Conference and Exhibition 2020, the EU Sustainable Energy Week EUSEW 2021, the European Materials Modelling Conference - EMMC 2021, the International Supercomputing Conference - ISC 2021, etc.

As an outbound action, in 2021 it organized a series of webinars, that aimed at presenting the flagship codes to a wide audience, pointing out especially the benefits they could give to materials modelling research at industrial level. The seven webinars ran from May to November 2020 and attracted a large audience of different levels of expertise. Below, a graphical representation of main results is given. More information can be found in the Webinar report booklet[3].

Furthermore, several actions were undertaken in collaboration with the CSA FocusCoE and other CoEs, by participating in specific working groups (e.g., WP3) and activities. We attended the FocusCoe sustainability workshops (5/11/2020 & 21/01/2021), in which all CoEs introduced their sustainability plans and discussed common strains. We contributed to the first workshop with a presentation on the "Sustainability plans @ MAX" (L. Neri, Cnr).

[3] https://zenodo.org/record/5109745#.Yv3mRC7P02w

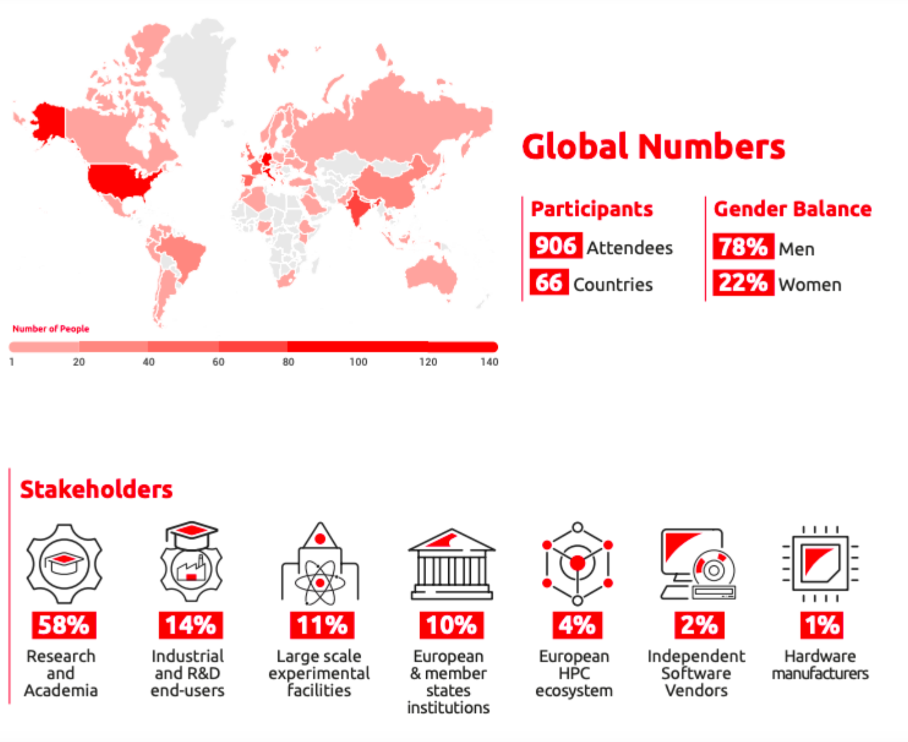

Fig 4. Global impact of the webinars (from the MAX webinar booklet, https://zenodo.org/record/5109745#.Yv3mRC7P02w).

3.4 Revenue

In general, software business derives 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 summarise the schemes identified in Ref. 4, and then describe the situation for MAX. The analysis is the same as from the Draft Business Plan, as it is still valid.

According to [4], 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 centred on open-source codes, which excludes *(b)* Subscription based software licensing. In (d) Open-source based business models, the main asset is the human knowledge/expertise. Therefore, 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 thus 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 standardised since 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 sales in terms of revenue and profitability (while experts can be charged per hour/day only once, 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 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 can thus be considered as a possible future business model for MAX, although not currently feasible.

(e) Government and public funding models are essential in the case of development of new software or major upgrade operations: it can take more than a decade to develop a code mature enough to be ready for industrial applications. In the D10.2 "Draft business plan: preliminary exploitation strategy" for MAX, the revenues were calculated considering limited or no funding from public entities, as recommended in previous reviews of the CoE. However, this exercise needs 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.

3.5 MAX Success Stories

As cited above in 4.1 Code section, MAX partners have stipulated several commercial contracts in these years. Among these, two success stories are showcased here, in order to present possible routes to commercialization.

Quantum ESPRESSO Foundation (QEF) and Schrödinger. The collaboration between the QEF and Schrödinger is a long lasting collaboration that mainly involves:

* regular meetings in which QEF provides technical support to Schroedinger scientists, who usually ask assistance about:
    - o the most suitable methodological and numerical approaches to study of some particularly problematic molecules and materials, that might be of interest for them or for some of their clients;

  - o assistance for the best ways to run calculations on some specific hardware (for example, how to run calculations on GPU, proper ways to exploit the different levels of parallelism implemented in QE);
  - o explanations about QE implementations, input keywords, output file formats, units of physical quantities printed in the output files;
- * implementing new features that are relevant for Schroedinger clients;
- * update the QE Schema with the new features that are from time to time added to new releases of the QE code.

SIESTA and SIMUNE Atomistic SL. The SIESTA code has shown a high potential for commercialization since its inception, which has been somehow dampened by the open-source approach adopted and the decision to make it free of charge for the academic community since its very first versions. However, the current GPL licence does allow for direct commercial exploitation, most effectively approached by maintaining the free software character of the core SIESTA code, but providing software products around it. This approach has been successfully followed by SIMUNE Atomistics SL, a spin-off company founded by some of the original developers of SIESTA (including Prof. P. Ordejón, ICN2, member of MAX). SIMUNE has built a business model for developing software products and tools around SIESTA. In particular, they have developed ASAP[4], a commercial product that includes an interactive GUI, structure builders, elaborated workflows to compute complex materials properties, and many analysis tools. ASAP is currently one of the main sources for income to SIMUNE.
Additionally, SIMUNE established years ago a long term commercial relation with the software company JSOL, from Japan. The agreement includes the distribution of SIESTA as part of the J-OCTA package for integrated multiscale materials modelling[5]. In particular, SIESTA is the quantum engine chosen by JSOL for J-OCTA. SIMUNE built the interface between SIESTA and J-OCTA, and obtains royalties for each licence of J-OCTA that includes SIESTA sold by JSOL. This relationship has also allowed SIMUNE to understand and become aware of the needs of the industrial users (mainly in Japan), which then they incorporate in their software products (mainly ASAP), increasing the value and commercial impact of its products.

4. Sustainability

In the D10.2 “Draft business plan: preliminary exploitation strategy” we analyzed different possible legal entities to make MAX act as a unique service provider, with no distinctions among partners. We presented different entity options, and prepared a three-year economic and financial plan in order to assess the possibility to set MAX up as a self-sustainable legal entity essentially based on commercial activities, including public funding deriving from national and international institutions and projects only at a marginal level.

We envisioned MAX as a legal entity capable of taking contracts related to materials modelling

[4] https://www.simuneatomistics.com/services/asap-software/
[5] https://www.j-octa.com/

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.

The new entity 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 partners, who should aim at strengthening the collaboration also through the commercial exploitation of the results, we drafted a three-year economic and financial plan [13] aimed at identifying the possible streams of revenues and 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.

The interest and role of the different MAX partners under these scenarios were assessed in the next two years, when MAX CoE continued to work 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. The revenues created by MAX partners in the entire life of the CoE were also assessed: even though there have been interesting interactions with industries, as shown in Appendix 1, the partners agreed on the hardness of a full-commercial sustainability path and preferred to pursue the way of a public financing for the third phase of MAX.

Even if a MAX entity essentially based on commercial consulting and service activities of great relevance to the European HPC ecosystem and economy would be probably sustainable beyond the end of the current H2020 funding period, it would be unable to sustain the research activities aimed at extreme computing and frontier innovation which are at its core, as they require long term investments beyond what could be sustained by commercial activities alone. A sustainable entity would thus pursue intrinsically different targets from the running CoE.

Discussion on sustainability options for CoEs was carried out also together with the other centres in the HPC CoE Council (HPC3) Business Working Group (WG) created by the H2020 project FocusCoE (CSA, GA Nº 823964) [14].
MAX partners benefitted from the initiatives organised by the CSA Focus CoE to support the sustainability planning of all CoEs, including training events with experts in the field of innovation

management and business development and interactive workshops. Finding ways to sustain CoEs operation after the end of the publicly funded project term is recognized as an important aspect related to the management of their potentiality in innovation.
The HPC3 report takes in consideration the organisational aspects related to the management of the business activities. The most basic relationship between two organisations (supplier/customer) does not apply to CoEs, that are consortia of several legal persons bound by an internal agreement to carry out a specific GA-DoA. The project partners are organised in different ways (universities, government-funded labs, commercial entities, …), and they have different capabilities and interests. What can be done is to establish such a relationship between a subset of partners on the supplier side and the customer, even if closing commercial-grade multi-party contracts is complex and both effort- and time-consuming. Three approaches were identified as effective for commercial exploitation: to act with a single partner, to found a legal entity, to establish associations with membership fees for the scientific or commercial customers.

In the second half of 2021, the HPC3 business working group launched a survey of the plans and experiences regarding innovation management, business development and sustainability among CoEs. 90% of the projects were expecting follow-on public funding, with 20% assuming that their operation would be fully funded from public sources. Amongst the commercial sources of income, consulting services and training lead by far; software licensing is only considered by 20% of the projects, with half of them also thinking about dual licensing schemes. Provision of software as a service (SaaS) and specific, licensed add-ons to software are considered by 30% of the CoEs. Concerning the costs, research for and development of the CoE software clearly accounts for the highest share of costs (73% on average), while training and user support come in second, with an average of 10%, followed by dissemination and outreach at an average of 8%. This might indicate a problem, since commercialisation of IP, services or software will likely require a higher amount of dissemination (indeed the need for marketing of the value propositions). Asked about which factors have been limiting their business development and sustainability activities, legal and funding constraints, lack of investors and insufficient clarity about potential market sizes are most often mentioned; lack of qualified personnel was mentioned by 20% of the respondents, and only 10% see the need to produce open source software as a limiting factor. 70% of the CoEs consider founding a non-profit organization, and 30% consider a commercial spin-off. In addition, 80% expect to continue as a consortium after the end of their term, probably anticipating follow-on funding.
It was recognized that core, fundamental scientific research on Exascale capabilities of codes will need substantial and continuous support from public funding grants. Still, there are opportunities for commercial activities which can supplement the research work.
A factor specific to the current CoEs is the funding agency’s emphasis on adapting applications and libraries to run efficiently on future Exascale systems. Achieving this objective will create significant value in the future, but the value of Exascale-ready codes for industrial end-users is limited at this juncture.
Given the relatively short-lived nature of projects like the CoEs (approx. 3 years), it is difficult to

build the required visibility and trust for software with a small user base, and thus guarantee stable long-term development. CoEs have to rely on long-standing governance structures for code development and maintenance independent of short-term project terms to become a successful market player. Acquisition of customers can take a long time and requires specific (non-scientific) expertise (on top of technical/scientific skills), in particular for the highly complex simulation codes typically developed by the CoEs. This further cuts opportunities.

Additional factors have to be considered before a business-to-business relationship can prosper: time-scales must be aligned; performing services for a commercial customer may be at odds with the personal goals of scientists; academic employment contracts are usually temporary with immutable terms; successful business development and customer acquisition requires specific "talents" and expertise which are not in the key skills set for domain scientists or expert software developers; the business value of the CoE software or service to the customer must clearly exceed the incremental costs incurred by the CoE.

Finally Focus CoE prepared a "*Report on Innovation Management Across All CoEs"*, where it provides a description, discussion, and analysis of the IPR and innovation management approaches employed by each of the ten EU HPC CoEs. All activities can be framed by the four-stage innovation management process, which includes: secure the foundations; capture project outputs; manage and protect project outputs; and dissemination, exploitation, and communication project outputs.

Among the seventeen key recommendations from the collective experience of the CoEs hence presented, the last three concern explicitly sustainability and are reported below.

Recommendation 15: If it is deemed that particular sustainability activities are incompatible with exascale scale development, then those particular sustainability activities should give way and/or be de-emphasised in order to ensure transition to the exascale. If development towards the exascale would struggle without additional public funding then this should be clearly communicated to the commission. This should not however prevent other sustainability routes being considered. If the CoE's DoA includes work on sustainability then this should be addressed, but the emphasis should be on the exascale.

Recommendation 16: *CoEs consider training and consultancy services as part of their sustainability plan, alongside other revenue streams they are able identify. Consultancy services in particular should not however be offered at the expense of the project research goals.*

Recommendation 17: CoEs should consider sustainability as early as possible within the project and develop, and periodically update, two sustainability plans based on polar financial outcomes. A hypothetical scenario where the project receives full funding for another iteration, and a hypothetical scenario in which it is not possible to obtain any additional funding. It is unlikely that either scenario will be the outcome of the project, knowledge and planning for the extremes however will make formulation of a final sustainability plan more straightforward.

Along these lines, a key development is that the sustainability of MAX will be guaranteed for the next four years by European fundings, as it is one of awarded CoEs in the "Centres of Excellence for HPC applications - HORIZON-EUROHPC-JU-2021-COE-01" call. This will permit it to

continue its activity in extreme computing and frontier research, and will make it able to take advantage of the entrance of new partners, e.g., HW manufacturers and a technology company. The CoE aims at not abiding to its commercial exploitation activity, though not compelled to it by sustainability.
The planned synergies with the National Competence Centres established by EuroHPC –as well as the coordination with the CASTIEL CSA– are expected to offer valuable opportunities for MaX exploitation activities within the European ecosystem.

5. Conclusions

This work updates the draft business plan through the analysis of the potential market on the basis of more recent literature, and updates the business model (value proposition, services, revenue) according to the last MAX contracts. The assessment on the possibility of setting up MAX as a self-sustainable legal entity essentially based on commercial activities has been discussed in the frame of recent discussion among CoEs in collaboration with Focus CoE and of a recent awarded European funding.
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 its core, as they require long-term investments beyond what could be sustained by commercial activities alone.

6. References

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5. EMMC-CSA – GA nr. 723867 Report on the Workshop on "Industrial impact of materials modelling", July 8-10, 2019, Turin, IT.

6. As an example, one of the surveyed modellers (Applied Materials IT) develops a proprietary code for interpretation of electrical characterization measurements and the reliability assessment of semiconductor devices.

7. Goldbeck Consulting Ltd, "The economic impact of molecular modelling: Impact of the field on research, industry and economic development", 2012. http://psi-k.net/docs/Economic_impact_of_modelling.pdf

8. This is a substantial upgrade to the numbers mentioned in the EU report "Materials Modelling: Where do we want to go?" Directorate-General for Research and Innovation, Key Enabling Technologies (NMPB) 2014 where the survey identified 16 commercial software owners.

9. N. Adamovic, P. Asinari, G. Goldbeck, A. Hashibon, K. Hermansson, and E. Wimmer, "EMMC Survey of materials modelling development needs: discussion notes towards the Road Map 2018-2020", 2016.

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11. G. Goldbeck (Goldbeck Consulting Ltd), "The scientific software industry: a general overview", Jan 2017. https://zenodo.org/record/260408#.Xd6Uf5P-2Uk.

12. A. Pinto, C. Sartore, Feasibility Study of a legal entity for MaX, November 2019 (confidential paper).

13. Report of the HPC CoE Council Business Working Group: "Sustainability for CoEs: Approaches, Successes & Lessons Learned", March 2022. https://www.hpccoe.eu/wp-content/uploads/2022/04/HPC3-WG-Business-Report.pdf

Appendix 1 - Industrial uptake.

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

Company	Website	Country	Sector
Applied Materials	https://www.appliedmaterials.com/	US / Italy	Manufacturing industry
ATOS	https://atos.net/en	France	Digital company
BIOVIA	https://www.3ds.com/products-services/biovia/	France	Innovation company
BI-REX	http://bi-rex.it/	Italy	Consulting
Bright Computing	http://brightcomputing.com/	USA	SW company
Clarivate Analytics	https://clarivate.com/	UK	Analytics for innovation
Comsol	https://www.comsol.com/	USA	Software vendor
Dassault Systèmes SIMULIA	https://www.3ds.com/products-services/simulia/?wockw=SIMULIA	USA	Modelling company
DYNAmore GmbH	https://www.dynamore.de/en	Germany	SW company
Exabyte.io	https://www.exabyte.io/	USA	Cloud-based software company
EXTOLL	http://www.extoll.de/	Germany	Semiconductor producer
Goldbeck Consulting	https://materialsmodelling.com/	UK	Materials modelling consulting company
Happy Electron Ltd	https://he.co/	UK	Energy innovation company
Hexcel Composites Ltd.	https://www.hexcel.com/	USA	Manufacturing company
Jeppesen	https://ww2.jeppesen.com/	Sweden	Aviation company
Johnson Matthey	https://matthey.com/	UK	Sustainable technologies company
Microsoft	https://www.microsoft.com/	US	Innovation and technology company
Moxoff	https://www.moxoff.com/	Italy	SW company

Company	Website	Country	Sector
Nokia	https://www.nokia.com/	Finland	Innovation and technology company
NVIDIA	https://www.nvidia.com/en-us/	USA	Accelerated computing company
Nyro Research India	http://nyro.tilda.ws/	India	Modelling company
Phasecraft Ltd	https://www.phasecraft.io/	UK	Quantum computing
QWED	https://www.qwed.com.pl/	Poland	EM modelling & research company
P4BUS Systems	http://p4bus.com/	France	Code developer for 3D printing
Pintail Limited	https://pintail.eu/	Ireland	Consulting company
RED Fluid Dynamics	http://www.red-fluid.com/	Italy	Research and development in fluid dynamics
Repsol	https://www.repsol.com/en/index.cshtml	Spain	Multi-energy provider
Robert Bosch LLC	https://www.bosch.us/	US	Manufacturing industry
Saipem	https://www.saipem.com/en	Italy	Technological and engineering platform producer
Samsung Electronics	https://www.samsung.com/uk/	South Korea	Electronics company
Sandvik	https://www.home.sandvik/en/	Norway	Manufacturing industry
Schott AG	https://www.schott.com/		Manufacturing industry (glass, glass-ceramics)
Schrödinger	https://www.schrodinger.com/	US	SW vendor
Sicos-BW	https://www.sicos-bw.de/	Germany	Consulting
Siemens	https://www.siemens.com	Germany	Technology company
SIMUNE atomistics	https://www.simuneatomistics.com	Spain	SW vendor
Simperler Consulting	http://www.simperler-consulting.com/Home_as.html		Scientific consulting company
SINTEF	https://www.sintef.no/en/	Norway	Applied research, technology and innovation company
Software for Chemistry & Materials	https://www.scm.com/about-us/	Netherlands	SW company
Solvay	https://www.solvay.com/en/	Belgium	Chemical company
Sony Europe Ltd	https://www.sony.net/	UK	Entertainment, Technology & Services company

Company	Website	Country	Sector
Stratec BioMedical Romania SRL	https://www.stratec.com/home	Romania	Manufacturing industry
ST Microelectronics	https://www.st.com/content/st_com/en.html	Italy and France	Electronics and semiconductor company
SUPERMICRO	https://www.supermicro.com/en/	The Netherlands	IT solution provider
Synopsys Denmark ApS	https://www.synopsys.com/	Denmark	IT solution provider
Tetra Pak Packaging Solutions	https://www.tetrapak.com/	Sweden	Food processing and packaging solutions
Toyota Central R & D Labs	https://www.tytlabs.com/	Japan	Transportation
Toyota Motor Europe	https://www.toyota-europe.com/	Belgium	Transportation
Umicore AG & Co. KG	https://www.umicore.com/	Germany	Materials technology company
VASP Software Gmbh	https://www.vasp.at/	Austria	SW company
Vinformax	http://www.vinformax.com/	UK	Innovation consulting company
VITO	https://vito.be/	Belgium	Consulting
Western Digital Technologies Inc.	https://www.westerndigital.com/	USA	Data storage innovation industry

Appendix 2 - List of commercial contracts by MAX partners in 2020-2022.

Source	Year	Type of service	Short description of the activity/service provided	Customer business area	Duration of activity / service (months)	Revenue (k€)
BSC	2018-2021	Code development	Code optimization	Hardware manufacturer	36	330
EPFL	2020	Materials discovery	Qubits	ICT		ND
ICN2	2019-2022	Consulting & training	Consulting about the use of SIESTA for the study of topological insulators	ISV	36	70