D4.3

First Business Plan

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D4.3 First Data Management Plan

Content

1. Executive Summary

One main goal of the INTERSECT project is the realization of a novel multi-scale multi-physics simulation platform connecting the materials modelling to the simulation of the electron device operations. The result will be the release of the Interoperable Material-To-Device Simulation Box (IM2D) which is conceived as an interoperable, robust and friendly software solution for easier exploration of the materials workspace from an electronic device-oriented industrial perspective. In particular, IM2D aims at enabling the simulation-aided design and optimization of devices for disrupting electronics (e.g. storage class memories, selectors, etc.), relying on the state-of-the-art quantum-mechanical materials modelling at the device level.
The beneficiaries of INTERSECT's IM2D platform will include the entire ecosystem of companies, research institutions and universities operating at various levels in the semiconductor field, including integrated device manufacturers, fabless semiconductor companies, semiconductors foundries, and R&D labs. In this huge playground the business opportunities associated with IM2D are twofold: (i) as a tool to increment the business of industrial stakeholders of semiconductor verticals; (ii) as a software product in the simulation software market.
As anticipated in the constituting Grant Agreement of the INTERSECT project, and confirmed in the consortium agreement between participant partners, "the project goal is the realization of a '*pre-competitive*' software solution that will provide the natural basis for start-up creation beyond the project end". Even though the final commercialization of the IM2D code goes beyond the aim of the present project, in this first business plan we thoroughly analyze the characteristics, the segmentation and the needs of the two reference markets (namely the semiconductor and the simulation software market). We will describe the solutions and the roadmap for eventually entering in these businesses. A detailed plan with a specific business model, a marketing plan and an analysis on the sustainability and future funding of the IM2D infrastructure – too premature at this development stage – will be described in the "Business plan assessment and revision" (deliverable D4.7), due at month 30.

2. IM2D solution for Semiconductor Market

In this section we analyse the main aspects of the semiconductor and synaptic electronics market, focusing on the specific characteristics that make IM2D a promising and robust research tool within the industrial R&D steps.

2.1 Semiconductor Market Overview

Electronics is nowadays pervasive in all aspects of our lives, covering consumer electronics, industrial automation processes and manufacturing, wireless communications, robotics, drones and transport, cloud communications, security and biometrics, automotive and domotics, just to cite a few. As such, the electronics industry plays a dominant role both in terms of macro-economic income (e.g. gross domestic product, market, employments) and in terms of social impact [e.g. social media, artificial intelligence (AI), internet of things (IoT)]. Since the world economic recession in 2009, the global semiconductor industry experienced a continuum positive trend. The world value of the semiconductor market was USD 481 billion in 2018 and USD 515 billion in 2019 and it is set to continue its robust growth well into the coming decade (see Figure 1, [1]).

However, despite the increasing global revenue, the eroding cost of electronic products along with the ballooning costs of infrastructures and goods are posing serious limitations to the competitiveness and the sustainability of many semiconductor companies. Most critical aspects are related to lack of innovation, inefficient manufacturing and testing of devices that reduce competitiveness and profitable growth [2]. The solution that leader companies embraced to solve this problem is the pursuing of a hybrid and flexible approach to manufacturing "from design to market", that is it requires the implementation of business processes and system capabilities able to optimize and support all aspects related to manufacturing including pre- and post-production (see below).

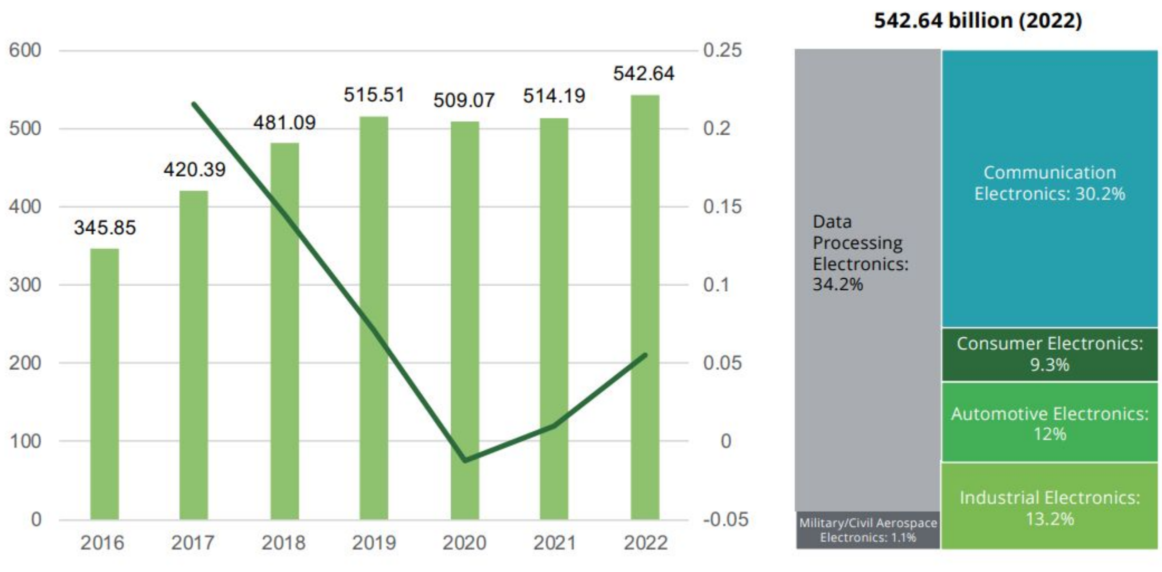

Fig. 1. Global semiconductor sales revenue from 2016 to 2022 (USD billion). Source Gartner, Deloitte analysis [1]

2.1.1 Segmentation

The global semiconductor market is segmented on the basis of the application, technology, and manufacturing. The right panel of Figure 1 shows the segmentation of the worldwide semiconductor revenue over the most important user applications. Data processing electronics (e.g. SSD storage and cloud computing) and communication electronics (e.g. wired and wireless) cover more than 60% of the entire market (Figure 2). The proliferation of PCs, smartphones, and cameras observed in the last 3-5 years rapidly saturated the market, dragging the total revenue of consumer electronics to less than 10% of the total amount. Industrial electronics (including security, automation, transportation, and energy management) and automotive sectors (e.g. ADAS, safety control, infotainment, navigation) are growing very fast (now 25%) and represent one of the driving forces for the future development of the semiconductor field.

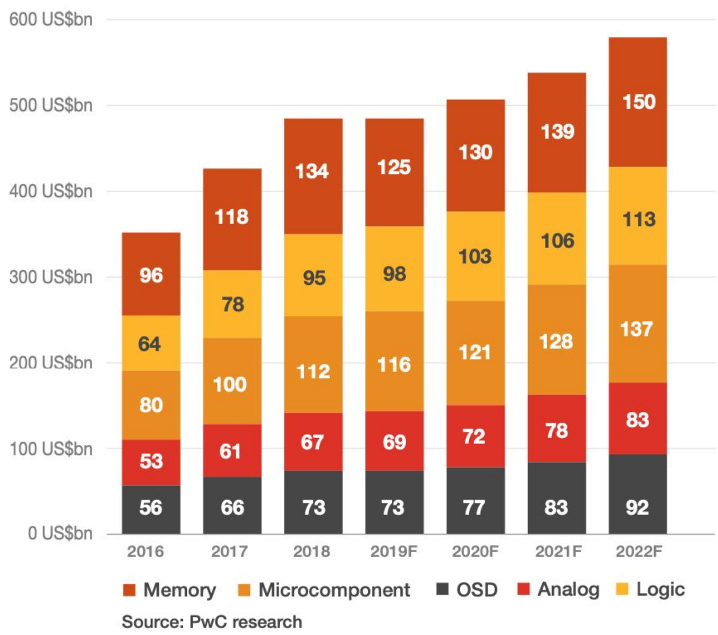

Fig. 2. Market growth by component type. Source PwC [6].

From the technological side, microprocessors represent nowadays the most important segment of the semiconductor market as they remain critical pieces of common electronic, automotive, computing, consumer, and media devices. However, the development of emerging technologies such as AI and IoT are hindering their growth and their leadership in the market. Optoelectronic, sensor and discrete components (OSD) are a fast-growing opportunity for the semiconductor industry, especially in the fields of automotive, domotics and security. The stand-alone memory market has experienced extraordinary growth over the past decade, driven by the increasing performance requests by cloud computing, AI, and IoT. NAND and DRAM account together for around 97% of the overall stand-alone memory market, and their revenues hit a record high of around USD 160 billion in 2018, registering an impressive CAGR of 32% between 2016 and 2018 (Source Yole Development). However, at the end of 2018, both NAND and DRAM markets started experiencing oversupply caused by unreasonably weak demand, including lower-than-expected smartphone sales and a slowdown in data center demand. This, along with a drastic decline of prices, remarkably reduced the role and the outlook of the memory segment for the next and mid-term future of the semiconductor market [4, 3]. Logic and analog components are demanded for communications, data processing, and consumer electronics sectors, assuring them a relevant and tendentially increasing part of the global market.

On the basis of manufacturing and production, the semiconductor market is divided into two main categories: semiconductor foundries and fabless companies. The former are factories where devices (e.g. chips, memories) are manufactured. The latter are companies that do not own a semiconductor foundry and do not take any part in the fabrication of the product but the designing, assembling and marketing aspects of the electronic system. The Semiconductor Foundry Market was valued at USD 42.03 billion in 2019 and is expected to reach USD 62.2 billion by 2025, at a CAGR of 6.75% over the forecast period 2020 - 2025 (Source: Mordor Intelligence [5]). A semiconductor fab owned and run by the company itself requires significant contributions in terms of capital, staff, and resource investment, as you would need adequate space, infrastructure, relevant equipment, skilled employees, and storage facilities to supplement the manufacturing process, not to mention the costs associated with the material and skill needed, waste disposal, and routine maintenance. The semiconductor foundry market is consolidated for a major share of the market is occupied by top players, such as Taiwan Semiconductor Manufacturing Company Limited, Global Foundries, United Microelectronics Corporation, Semiconductor Manufacturing International Corporation, Samsung Group, Dongbu HiTek, Fujitsu Semiconductor Limited, STMicroelectronics.

Fabless companies represent an alternative model to semiconductor foundries. The characteristics of fabless companies is to outsource the manufacturing of semiconductor chips to an external supplier. Such a business strategy allows the fabless companies to avoid high capital and resource investments and to focus their time, efforts and resources on developing new ideas, investing in research, and improving their marketing strategies to drive their sales. This business model also favors a high variability in production volume, efficiency, and velocity without feeling an overburden on their staff and resources. In 2018, fabless companies have globally made revenues of USD 100 billion. The estimated contribution from these companies to the semiconductor industry is expected to be higher than 50%. Companies such as Qualcomm, Broadcom, AMD, NVIDIA, Xilinx, Marvell, and MediaTek are some of the major names in the fabless company realm in terms of the number of sales made and the total revenue generated.

If we consider the market size by region, the Asia Pacific region will remain the world's biggest market for semiconductor consumption with a CAGR of 4.8% through 2022 (Figure 3). The American region will draw the second-highest CAGR over the forecast period at 4.3%, propelled largely by projected gains in the market for NAND flash memory chips. In this region, the US is home to a number of leading semiconductor companies and has a strong startup ecosystem. EMEA will draw a CAGR over the forecast period of 3.5%. Europe's ambition is to attain a 20% world market share in the semiconductor industry. In fact, for many European industries and applications, semiconductor content is essential. Europe has leading companies in a number of sectors like automotive, mobility (rail, air) and engineering. In order to increase the EU market share and open new channels of profit, it is necessary to invest in innovation.

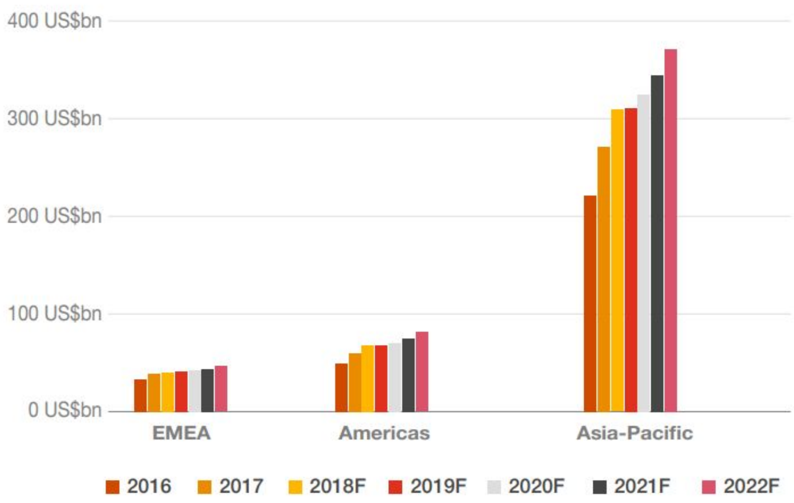

Fig. 3. Semiconductor revenue by region. Source PwC [6].

Most semiconductor foundries are located in the Asia-Pacific area (e.g. Taiwan, Korea, China) and in the US, while fabless companies are often headquartered in costly, industrialized countries, including the US and Europe.

2.2 Synaptic electronics and Neuromorphic Computing Market

The need for innovation and emerging of novel technologies such as IoT or AI have fostered the development of novel and disruptive solutions. In this regard, synaptic electronics and neuromorphic computing are emerging as promising and robust verticals from the vast landscape of the semiconductor market. The idea at the basis of neuromorphic technology is to implement aspects of biological neural networks as analog or digital copies on electronic circuits. The goal of neuromorphic computing is twofold: (i) to offer a tool for neuroscience to understand the dynamic processes of learning; (ii) to apply brain inspiration to generic cognitive computing. Synaptic electronics enable a machine to learn, adapt and function as a human brain does rather than functioning as a normal computer. As such, neuromorphic computing is expected to gain huge momentum in the coming years due to the rising demand for AI and machine learning for application fields such as language processing, computer vision, and image processing, real-time data streaming, and cognitive robotics.

Neuromorphic chips exhibit qualities such as low power consumption, high-speed accuracy, and optimum memory usage. Global Neuromorphic Computing Market was valued at USD 42.08 Million in 2018 and is estimated to reach a market value of USD 648.40 Million by 2025 growing at a CAGR of 49.92% during the forecast period 2019–2025 [7]. However, limited research and development in this market due to huge investment and advanced technologies required, coupled with complexity in the designing and manufacturing of neuromorphic chips are the major factors inhibiting the growth of the neuromorphic computing market.

The key players of the global neuromorphic computing market are Brain Corporation, CEA Leti, General Vision Inc., Hewlett Packard, HRL Laboratories LLC, IBM, Intel, Knowm Inc., Numenta, Inc., Qualcomm Inc., and Vicarious FPC, Inc.. However, a plethora of new SMEs and startups (e.g. Aspinity Inc, aiCTX AG) have taken advantage of this emerging field, and now offer neuromorphic hardware processors which aim to improve AI-based and neuromorphic computing applications.

2.2.1 Segmentation

The market for neuromorphic computing is segmented on the basis of application, offering, and industrial verticals (i.e. end-users).

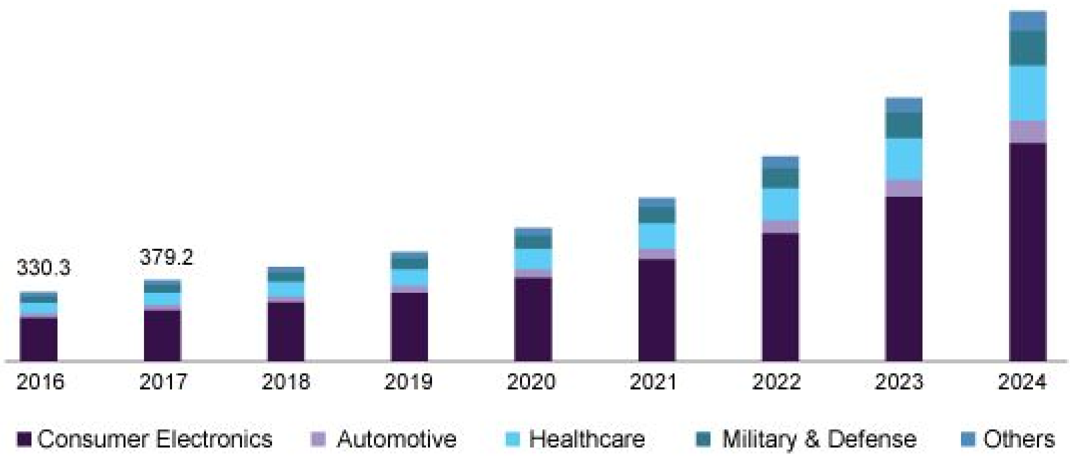

Fig. 4. US neuromorphic computing market size, by end-use, 2016-2024 (USD million), Source Grand View Research [8].

Neuromorphic computing has a wide range of applications such as image recognition, signal recognition, data mining, object detection, and many more. Sorting by the end-user, the market can be split into five segments: automotive, consumer electronics, military & defense, healthcare, and others (Figure 4), with the consumer electronics expected to hold the largest share in terms of end-use application. The usage of neuromorphic computing in self-driven and smart vehicles is expected to bring a transition in transportation and furthermore propel the growth of the automotive sector. Moreover, the usage of neuromorphic chips in satellites for surveillance and aerial imagery is highly in demand in the defense sector.

On the basis of offering, the segment is further classifiable into hardware and software. Software for neural network control is expected to hold the largest share of the neuromorphic computing market. More relevant for the purpose of the INTERSECT project is the hardware side, where storage-class memory elements (such as memristors, PCM, FeRAM) represent the largest and most promising sector of this market. Global memristor market was valued at USD 3.2 million in 2015 and is expected to reach USD 79.0 million by 2022, supported by a CAGR of 69.9% during the forecast period 2016 to 2022 (Source Allied Research [9]). In a similar way, the global PCM market is forecast to reach USD

46.52 billion by 2026 (Source Reports and Data [10]). The worldwide market for FeRAM is expected to grow at a CAGR of roughly 3.7% over the next five years, so to reach USD 300 million in 2024, from USD 240 million in 2019 (Source Transparency Market Research [11]).

PCM and FeRAM are considered prominent emerging technologies since they have the potential to provide cost-effective, high-density, high-speed, and high-volume nonvolatile storage on an unprecedented scale. In particular, PCM technology is ideal for both non-volatile dual in-line memory modules, and non-volatile memory expresses solid state drives. The technology is also much more durable than flash, and the concern of wear-out by daily writes is also not an issue.

Storage class memories are particularly relevant for the present project, as they are selected use-case applications for testing the proposed IM2D software (see below).

The region dominating the global neuromorphic computing market is North America: US and Canada are holding a major share in the global neuromorphic computing market. The leading player in this market growth is the image recognition industry. The growing demand for automation in countries such as South Korea, China, Brazil, and India is triggering the global market growth in the Asia-Pacific and the South American regions. Europe held a market share of 23% in 2018 and is forecasted to grow with a CAGR of 89.3% by 2026 [10]. The European market is also gaining momentum owing to the rise of opportunities for neuromorphic and AI projects.

2.3 Market needs and priorities

2.3.1 R&D investment, costs, and efficiency

Semiconductor companies today must be more rapid and agile than ever to remain competitive. As shown in the KPMG Survey (Figure 5, [13]), the key point for innovation is increasing the investments in R&D. The top 2500 Scoreboard companies invested in R&D USD 741.6 billion in 2016/17 (18% of revenue), an increase of 5.8% with respect to 2015/16, following an increase of 6.8% in the year before [12]. Companies also raised significantly operating profits (8.7%) and more modestly the number of employees (1.7%). In contrast, they showed an important decline in fixed capital investments, stagnation in revenue growth and a modest increase in the number of employees. Despite revenue growth fluctuations, R&D costs continue to rise, particularly on the leading edge. As a consequence, 78% of companies expect their R&D spending will increase in the next 2020, and nearly 30% of respondents reported they will invest more than one-quarter of this year’s revenue in R&D (Figure 5). So far, the main response has been incremental improvements to the traditional approach to R&D and more recently a wave of consolidation through M&A that has allowed companies to scale their R&D across broader revenue streams.

Fig. 5. Top strategic priorities for semiconductor companies over the next three years. Global Semiconductor Industry Survey, 2019. Source KPMG [13].

On the other side, the increase in R&D costs represents also the main issue for industry development and sustainability (Figure 6). Other expected issues, including cross-border regulation like new trade policies or tariffs, and talent development management, are affecting semiconductor industries' business. For SMEs which R&D is their reason for being, costs to execute innovation and talent retention are a big deal.

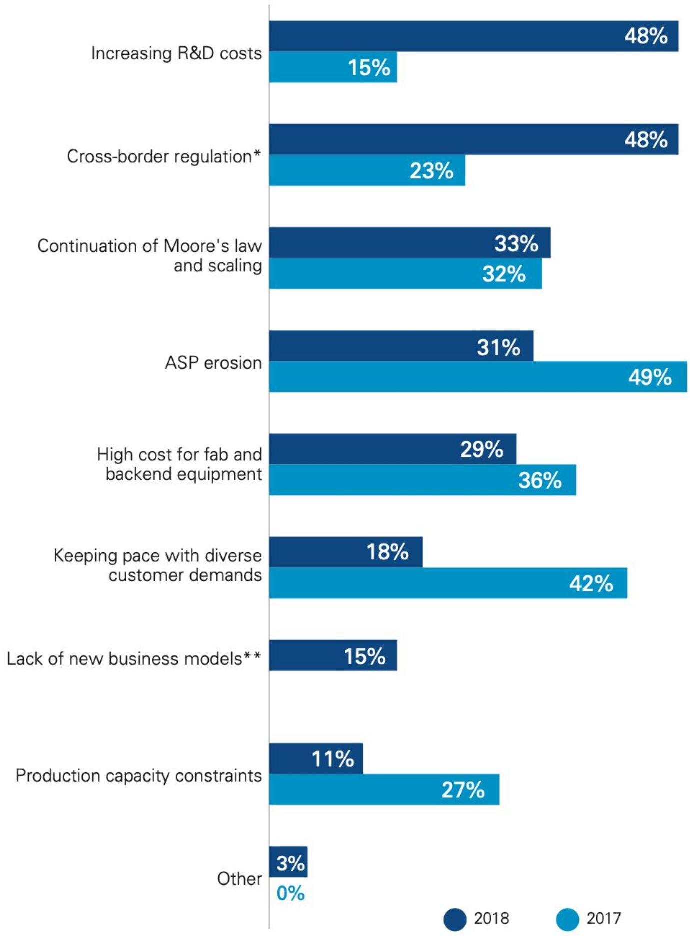

Fig. 6. Main Issues for Semiconductor Industry during the next three years. Source KPMG Survey, 2019 [13].

The most prominent cost in R&D expenses is that of personnel: the ratio between staff, software and hardware costs is 100/20/6, respectively. In the case of the production of a chip, for example, this implies an R&D staff cost of about 150K€-300M€, that is about 100K€ per engineer. Team sizes can range from 3 (startup) to 1000 (Intel) engineers. In perspective, the increase in the R&D costs is going to be sustainable only by big companies.

Despite the amount of R&D investment, semiconductor companies report high-failure rates of R&D programs. This is often due to deficiencies in initial planning, inability in adapting R&D plans to new market needs or accidents, low integration with pre- and post-production steps. Application of methodologies, such as the *Agile*, that can yield tremendous value to the semiconductor R&D planning and product development process. Further, the integration with D&A might help increase R&D efficiency not just limited to the cycles of continuous integration. Leveraging effective D&A helps unlock insights into improving R&D processes. This is confirmed by several dedicated analysis on R&D improvements [14,1] indicate that the use of data-driven insight and real-time analysis speeds up delivery time, helps change mindsets, and allows companies to tackle more complex projects. Moreover, using data as a basis for decision-making can avoid communication barriers between design teams and process teams.

R&D efficiency is challenging for companies of all sizes. SMEs may lack formalized processes for spotting and valuing high-potential innovations and may be more likely to fund doomed products. However, as they grow, sizable, highly diversified companies may lose the visibility and control over investments that small firms with just one or two products in the pipeline enjoy. This is driving established companies to make corporate acquisitions a larger part of their growth strategies.

2.3.2 Talent development

"Talent is a top-three or top-five problem facing the semiconductor industry. Anything else, if we get the right talent, is solvable". Dan Durn, Senior vice president, and chief financial officer Applied Materials Inc..

Innovation, implementation of disruptive ideas and efficient R&D requires the work of a large and interdisciplinary team, which includes material scientists, device architects, logic designers, verification engineers, etc. The research of talented personnel poses a serious problem in the development and the competitiveness of semiconductor industries (Figure 5). According to a recent analysis from Deloitte and SEMI (Figure 7), several companies sadly report difficulty in finding highly-qualified positions, in particular electrical engineering (60%), computer sciences/software engineering (35%), mechanical engineering (35%), computer systems/engineering (30%), and materials sciences/chemical engineering (30%).

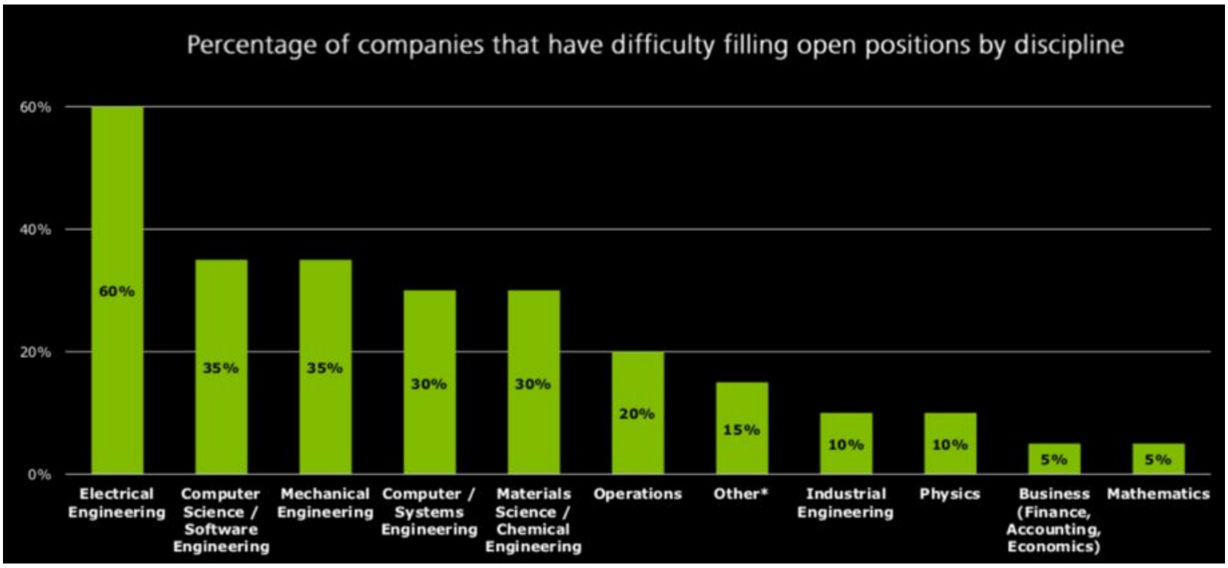

Fig. 7. Engineering Talent Shortage. Source Deloitte [1].

The talent competition is fierce, and big companies are usually advantaged in this competition. Small companies and SMEs often are not able to cover all the requested expertise in the design, fabrication, and test of electronic products, and suffer the lack of high-level skills.

The industry-wide shift to a more service-oriented business model also contributes to the perspective on talent risk. Recognizing that components can be commoditized, many semiconductor businesses are investing in software and related services to build more holistic, platform-based solutions that meet a broader range of customer needs.

2.4 The IM2D solution

2.4.1 Mission

INTERSECT mission is to exploit the synergic interplay among material and device simulation tools to reduce the gap between ideal and "real-life" materials, for direct and easy exploitation by industrial users. Our action is dedicated to pursue and accelerate the design of advanced complex materials and innovative devices for application in emerging electronics (e.g., synaptic electronics and neuromorphic computing), with the explicit intent to support and develop the competitiveness of semiconductor companies, including SMEs or startups (especially in Europe) that may suffer the competition with electronics giants from US or Asia.

2.4.2 Concept and value proposition

The development of new electronics requires the engineering of emerging nanodevices. This process is based on two main pillars: i) characterization/design of materials and ii) characterization/design of devices. Albeit implicitly interconnected, the interplay between the parameters that characterize the materials (e.g. structure, composition, doping, stability, electrical and thermal response) and the influence they have on the device (e.g. data retention, power consumption, interconnection, switching time) is hard to determine. This calls for the investigation of *materials at device level*: the study of materials in their general, device-independent, aspects or of their scaling down to nanoscale is not sufficient for such advanced device applications. Rather, atomic-scale material properties, temperature response, charge, and ion transport phenomena need to be incorporated into a device level description allowing to handle technology issues, device geometry, integration and biasing scheme. In other words, the characteristics of the material are inherently connected to the device performance requirements. Achieving such a direct link is a tremendous challenge for industrial users that requires a huge amount of time, material and personnel consumption, advanced technical skills, data analysis, and thus high costs (see above).

Materials modelling can efficiently contribute to this process by reducing the experimental trials and fostering efficient top-down and bottom-up design paradigms. Materials models and software tools have achieved a high level of stability and resilience enabling their direct use in numerous industrial applications and commercial software tools. When integrated into the industrial BDSS, modelling is demonstrated [19] to produce clear economic impacts and becomes an integral part of product life-cycle management in industry, supporting all steps of the production stage from research to manufacturing.

From the modelling side, unraveling the interplay between materials and device performances requires unprecedented capability of simulating and calculating properties of complex materials well beyond the standards the typical industry-driven software, which are optimized to model complex devices and circuit architectures, provided that the characteristics of the material in the device configuration are available (existing phenomenological and validated models and assumptions, existing constitutive relations i.e., material relations, etc.). This calls for the use of more sophisticated modelling solutions (e.g., based on atomistic quantum mechanical models) able to catch the complexity of advanced materials. Albeit very powerful, this software is usually developed in academic research groups and is not industry-driven. The generation/analysis of simulations and data requires advanced specialized skills that are not easily available to industrial end-users, especially to SMEs with limited R&D resources (Sec. 2.3).

In this regard, INTERSECT is an interdisciplinary project for the realization of an advanced industry-driven simulation box (IM2D) for emerging disruptive electronics. Starting from a set of stand-alone models and codes relevant to disruptive electronics, IM2D conjugates the advantages of both material and device-driven software, connecting the properties of materials at the atomistic level to the electrical behaviour of devices, including variability and reliability at the statistical level. The result is an interoperable, automated, and integrated simulation box that allows the user to manage codes, calculations, and input/output, and to establish the dynamical paths and causes/dependencies among data and simulations, i.e., controlling the modelling pipeline among the entire ecosystem. A simplified scheme of the IM2D infrastructure is shown in Figure 8.

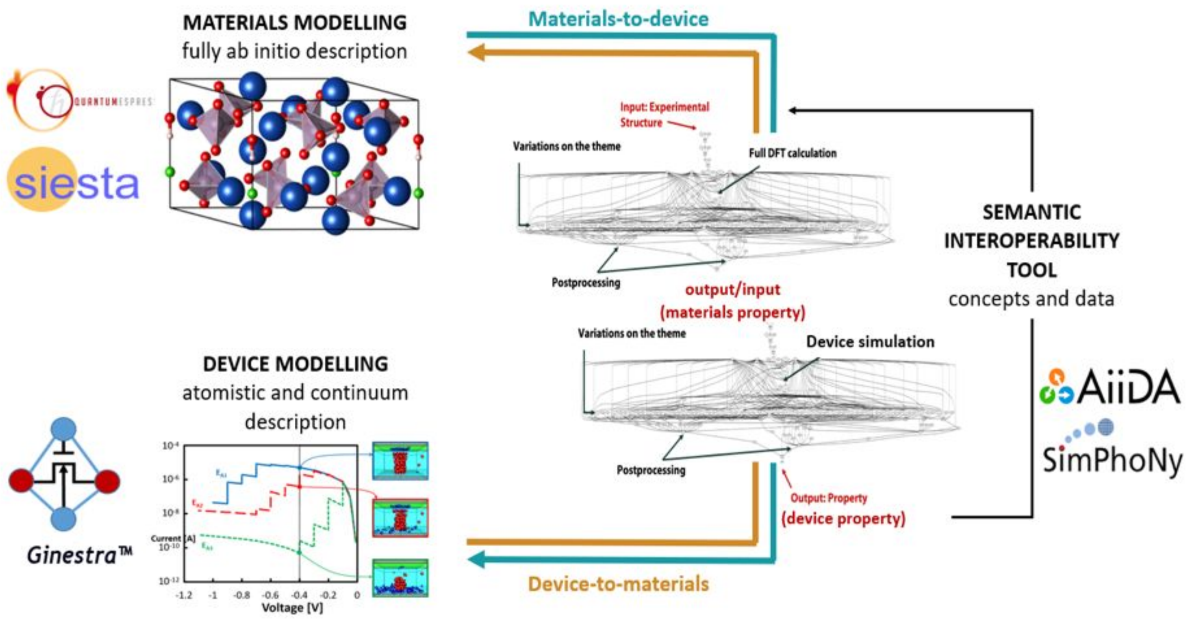

Fig. 8. Scheme of IM2D infrastructure.

The core of materials simulation is realized by Quantum ESPRESSO and SIESTA that are among the most widely used tools for quantum mechanical material modelling, while device modelling is provided by proprietary software Ginestra™, which is based on device-oriented continuum model and designed to simulate the electrical response of a selected synaptic devices (e.g. FeFET, selectors, PCM, RRAM, etc). All original stand-alone software will be integrated, with an increasing level of interoperability, by exploiting the capability of the SimPhoNy and AiiDA infrastructures: SimPhoNy provides the front-end for interoperability while AiiDA provides the infrastructure for data provenance, job management, and workflow execution. IM2D is conceived on two main cycles, namely materials-to-device and device-to-materials (Figure 8), which allows for a top-down and a bottom-up approach to device optimization. The combination of physics-based modelling with the data-driven approaches is an added value that makes IM2D a unique product for the semiconductor industry needs and the demands of the Materials Modelling Market.

2.4.3 Towards the semiconductor industry's needs

IM2D is a common platform that allows for the exploration of the materials using a device and product-oriented approach that is urgently needed by industry.

Responding to the market needs of R&D efficiency improvement, IM2D aims at reducing the overall development time. Expected IM2D impacts include more efficient experimentation, a broader exploration, and deeper understanding and saving a product development project and/or accelerated product development. The IM2D (meta)data can be exploited by end-users for a direct comparison with experiments or as input for other industrial simulation tools in the generation of a hierarchical code chain for the modelling of multilevel architectures or circuits. This means a significant reduction of screening by experiment and a minimization of the lab tests, with a consequent reduction of the costs. As Glenn Jones and Johnson Matthey declared during the EMMC workshop on "Industrial impact of materials modelling" (Torino IT, 2019), the economic impact of Materials modelling in R&D has a ROI of 8 and impact 5% of sales spent on R&D.

As shown in the previous Section, there is an urgent need for talents. The high level of interoperability constitutes a net forward in the simplification and automation of the simulation process, shifting the complexity of the problem from the front-end level and thus reducing the level of expertise required by the industrial user. The end-users (R&D staff, scientists, application scientists) will have thus access to high-level technical quality attributes for developing innovative electronic devices.

On the other side, IM2D will help to bring materials modelling to the heart of industrial business decision-making levels, allowing industry to rapidly build custom-designed integrated materials modelling apps and data-driven business decision systems, reducing the costs and time to market. Indeed, IM2D can be integrated readily in BDSS to assist rapid and efficient decision making:

- **Determining the essential data points.** Prior to interpretation the IM2D analytics platform will define what data points are most critical at each milestone in each product development process. This complex logic will later synthesize and give overall view of the status, quality, and development costs of an entirely novel device.

- **Establishing an agnostic and adaptable platform** to gather essential data, make a predictive analysis, and drive business decision making.
- **Establishing a baseline**. Using IM2D solution, the companies will be able to establish their baseline of current state performance. Data gathered from baselining can then be used for future continuous improvements and process optimization.

All these aspects contribute to accelerate the implementation of innovative technologies and unlock the potential of semiconductor, EDA and other addressable markets. Summarizing, by integrating IM2D solutions into their R&D processes, semiconductor companies can reduce costs of development of new products for the semiconductor market and can improve their position for a competitive advantage, increasing:

- **Time to market**: Shortened design, continuous integration, and validation cycles enabled by IM2D platform.
- **R&D strategy**: Cost-savings, more efficient use of R&D resources, and prioritization of the most important programs, especially within R&D management methodologies (e.g. Agile).
- **R&D staff**: High automation and semantic interoperability level of IM2D contributes to reducing staff cost and the talent risk.
- **Development process:** IM2D contributes to increasing the productivity empowering faster cycles of learning generated from the design databases across various teams and locations.
- **Innovation**: Materials discovery capability of IM2D allows an easier exploration of the material workspace from an electronic device-oriented industrial perspective.
- **Integration**: Close integration with pre- and post-manufacturing steps for two-way data exchange (material-to-device and device-to-material) for device optimization.
- **Decision making**: End-users can gain greater insight into risk and delays, enabling proactive decision making to manage resources and customer commitments.

3. IM2D and the simulation software market

In this section we analyze the perspectives of IM2D software to penetrate the simulation software market as a commercial product. We will focus in particular on the materials modelling market and its needs.

3.1 Simulation software market

The global software industry consists of three main sectors, programming services, enterprise software products, and shrink-wrapped software products. As the technological opportunities came into big numbers and the scope for the business environment started to flourish, these three sectors became established. For the purposes of this document, we focus only on shrink-wrapped software products and on simulation software, in particular.

Simulation software is a program that allows companies to create an in-silico process and observe an operation without actually performing it. It enables testing the same or modified system with different inputs, tracking, and analyzing responses. Simulation software is used widely to design equipment so that the final product can be close to the design specifications without being expensive in-process modification. Numerous companies in pharmaceutics, biotechnology, chemistry, aerospace & defense, and automobile sectors have invested heavily in research to develop image recognition and related applications [20]. The global simulation software market was valued at USD 8.24 billion in 2019, and it is expected to reach USD 16.00 billion by 2023 (Figure 9). The market is expected to witness a CAGR of 16% during the forecast period (2020-2023). The simulation software provides a rich training experience to the user for various end-user applications without using any physical asset and loss to the company, which is primarily the major reason to boost the market growth over the forecast period. (Source Market Research Future [21]).

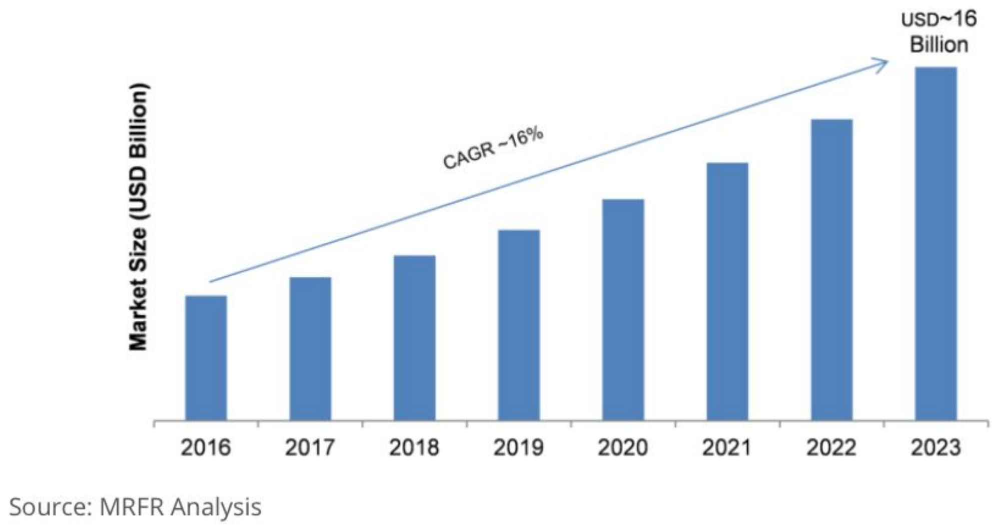

Fig. 9. Global Simulation Software Market. Source Market Research Future [21].

The rise in demand for an eco-friendly work environment, the need for creating and simulating models that are less expensive than producing and testing hardware prototypes, and the increase in the use of simulation software in the automotive industry drive the growth of the global simulation software market. In addition, an increase in focus on R&D activities (see above) and significant adoption of simulation among aerospace and defense are expected to provide lucrative opportunities for the growth of the market. However, risks associated with data security of simulation software are anticipated to hamper the market growth during the forecast period. Emerging trends such as digital twins in the industry 4.0 and the use of simulation software to develop IoT and AI supporting devices are expected to provide lucrative opportunities for the global simulation software market during the 2020-2025 period [22]. The global simulation software market is dominated by key players such as Altair Engineering, Inc.; ANSYS, Inc.; Autodesk, Inc.; Bentley Systems; Dassault Systems; Hexagon (MSC Software Corporation); The MathWorks, Inc.; PTC, Inc.; Siemens PLM Software; and The AnyLogic Company.

3.1.1 Segmentation

The global simulation software market is segmented by component, deployment, application and vertical. On the basis of components, the market is segmented into software and services. In 2016-19, ‘finite element analysis’ captured a lion’s share in the global simulation & analysis software market owing to growing application of software in various end-use industries including automotive, aerospace & defense, etc., and the segment is anticipated to maintain its dominance over the coming years. The second-largest share was held by ‘computational fluid dynamics’ due to its usefulness in designing and analyzing energy-efficient devices like heating, ventilation and air conditioning systems, thermal power plants, etc., besides allowing engineers and scientists to perform computer simulations or numerical experiments in a ‘virtual flow laboratory’ [23]. The ‘services’ segment is further classified into design & consulting and support & maintenance. Based on deployment mode, the market is bifurcated into on-premise and cloud. Based on the deployment model, the on-premise segment led the simulation software market in 2017. However, the cloud segment is expected to witness the highest growth, as product complexity, need for agility and collaboration drive the cloud-based simulation software market adoption.

Based on the application, the market is segmented into eLearning, training and research & development and others. Whereas, based on vertical, the market is segmented into automobile, aerospace and defense, electrical and electronics, industrial manufacturing, healthcare, education & research, and others.

Driven by the growth of the automotive market, the global simulation software market was led by the electronics and electrical sector in 2017 and is projected to maintain its dominance during the forecast period. However, the aerospace and defense sector is anticipated to witness the fastest growth, registering a CAGR of 13.30% during the forecast period.

The North America region holds the largest share of the market across the globe (42%) followed by Europe (30%), and Asia Pacific region (28%, Source Markets&Markets). US and Canada are dominating the North America market due to rising technological enhancements and growing adoption of simulation software solutions in the region. Moreover, the region has a well-established infrastructure, which allows for faster implementation of advanced technologies. Additionally, the growing adoption of simulation software solutions across industry verticals such as healthcare and manufacturing is another major factor driving the growth of the simulation software market in the region. On the other side, Asia-Pacific region is expected to be the fastest developing region for the overall market during the next 5 years. The increasing industrialization coupled with the expansion of various end-use industries is expected to boost the growth of the overall market. Additionally, increasing government initiative is also driving the simulation software market in the region.

3.2 Materials Modelling Market

Materials Modelling is the segment of the simulation software field explicitly dedicated to characterization, discovery, and design of materials and compounds. Despite the increasing diffusion, only a few data are available on the MM market analysis.

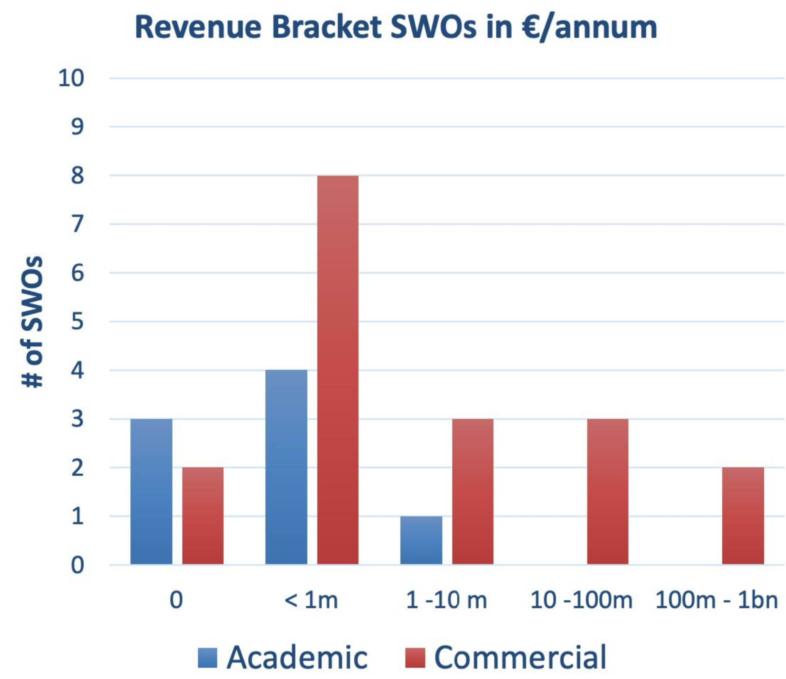

Fig. 10. Revenue Bracket in €/annum Source [24].

One cause of this lack is the relatively small user community (with respect to the global software users): the number of users of scientific software, such as molecular modelling in physical/chemicals/materials, is in the range of a few thousands in industry and a few tens of thousands in total. Another relevant cause is that only a fraction of the MM software is distributed through commercial licences. In fact, most of the MM software has been developed in universities or academic research centers and distributed as open source codes, free of charge. Figure 10 [24] shows the revenue distribution of most relevant SWO. The largest number of commercial SWO falls into the bracket of less than one million Euros per year. In the case of academic SWO, no income means that their software is distributed for free. As in the commercial case, most academic SWO also fall into less than a million Euros bracket. For academic codes the evaluation metrics for software are usually defined in terms of scientific publications, citations or data generation, rather than in economic revenue. Recently Ghiringhelli and coworkers [25] proposed analytic criteria to classify and standardize electronic structure codes (including Quantum ESPRESSO and SIESTA) and their performances. Other analyses on the MM market and the description of stand-alone codes are provided, e.g., by MaX (Material design at the exascale), EU Centre of excellence www.max-centre.eu.

3.2.1 Segmentation

MM software market is segmented on the basis of production stage, value chain, application, model. MM software can be classified in terms of value chain [24] in design “with” a given material and the development of “the” material itself. The estimated market of the former is about USD 4 billion with a CAGR of 1%, while the market share of the latter is limited to USD 100 million. In the specific case of disruptive electronics (i.e. market with high level of innovation) the limitations on the development of novel materials with tailored properties are one of the most important issues in the development of brand new technology. The discovery capability of the IM2D platform to search novel complex materials aims explicitly at fulfilling this need.

The relevant industry sectors that depend strongly on materials innovation are materials science, pharmaceutical and biotechnology, chemistry, and electronics. More generally material development and design are strategic for several industry verticals such as automotive, aerospace, transport, telecommunication, packaging, adhesives, healthcare, textile industries, etc. [20].

MM solutions can further be classified in terms of the implemented models, in particular data-based versus physics-based modelling. Data-based models are at the basis of most data-mining and machine learning approaches to research, i.e. they exploit data to generate other data or knowledge. The physics-based models use knowledge to generate data or other knowledge. Physics-based models are classified also by the entity type described (electronic, atomistic, mesoscopic and continuum). A detailed formalization and classification of most relevant models, physical equations and materials relations can be found in the Review of Material Modelling (2017) [26]. Cheminformatics [27] is the most relevant market area; it is mainly focussed on drug discovery but includes players also active in software for discrete (electronic/atomistic/mesoscopic) materials modelling, and Computer-Aided Engineering (CAE). The Continuum Materials Modelling Market (such as FEM or CFD related) is part of the CAE market and estimated in the region of at least € 1 billion. At the moment, software that can handle or contribute to solving multi-scale and multi-physics problems has high demand on the Materials Modelling Market. Additionally, development of unique algorithms and combination of physics-based modelling with the AI/ML data-driven approach would help you to find one’s niche in the modern materials modelling software market.

In contrast with the general trends on semiconductor industry or global software market, Europe has a leading role in development and implementation of materials models and scientific software tools (e.g. Quantum ESPRESSO, SIESTA, Fleur, Exciting, Abinit, CP2K, VASP, YAMBOO, Octopus, CPMD, wannier90, WanT, Gromacs, MolD, FHI89md, etc).

The European Community has fostered several initiatives to support and develop the scientific computing in both academic and industrial sectors through, for example, funded collaborative projects (e.g. INTERSECT), or initiatives like E-Infra Centres of Excellence such as MaX (Material design at the exascale, www.max-centre.eu) or PRACE (Partnership for advanced computing in Europe, http://www.prace-ri.eu). In the specific field of materials modelling, EMMC mostly contributed to coordinate all existing activities in Europe, with the aim to promote the integration of materials modelling into the state-of-the-art industrial BDSS.

3.3 Interoperability and Standards

Solution of complex problems (e.g., production of new technology) requires the combination of advanced knowledge and state-of-the-art technologies, often maturated in years of R&D and belonging to interdisciplinary areas. This implies the integration of technologies, platforms, protocols, and schema originally developed and implemented by different communities with different languages and purposes. Since these solutions are already in place, it is practically impossible to replace one or more of them to achieve a joint and coherent system. Hence, by casting knowledge into unambiguous and machine-processable data structures, interoperability is the natural route of choice to allow different stakeholders to access technology and interpret data unambiguously. By enabling interoperability, technologies can support the seamless integration of data from different sources to create complex environments able to carry innovation leaps. However, albeit well established in communication technology and IoT interoperability is an emerging concept in materials modelling and electronics modelling, limited to the structural or syntactic interconnections among physical models and codes, e.g. coupling-and-linking of models and the generation of a data pipeline between existing codes.

The need for automation and integration asks for interoperable solutions that go beyond the compatibility among models and codes. Implementation of semantic interoperability allows for the description of the information meaning in a formal and machine-readable and processable way (metadata and schema based on semantics). In this way, semantic interoperability generates interdependence between concepts and data: concepts provide the meaning for a set of data, and datasets cannot be exchanged without a linking concept that describes their meaning.

However, semantics alone is not sufficient to solve the problem of heterogeneity if players follow different definitions. This fundamental issue can be solved by adopting a shared ontology (including core vocabularies and standards). By means of a formal and explicit specification of shared concepts (e.g. material entities, models, materials relations), ontology promotes a common understanding of a domain, provides a reference terminology and a standardized classification of materials models and related metadata, as well as represents knowledge as a set of concepts related by hierarchical relations [28].

The use of common standards based on ontology is the prerequisite for a structured approach that includes generation, analysis, storage and re-use of data. This is also a fundamental request for any data-based research approach.

Very recently, EMMC provided a unified European Materials Modelling Ontology (EMMO), aimed at the development of a standard representational ontology framework based on current materials modelling and characterization knowledge. Instead of starting from general upper level concepts, as done by other ontologies, the EMMO development started from the very bottom level, using the actual picture of the physical world coming from applied sciences, and in particular from physics and material sciences [29].

3.4 IM2D and the Materials Modelling Market

IM2D is an industry-ready integrated, standardized, interoperable software solution which stems from multidisciplinary experiences in the fields of physics, material science, electronic engineering, and informatics. IM2D provides the upscale of software of both academic SWO and commercial companies and accelerates the uptake of material modelling in European industries by establishing an intermediary translation process. The IM2D platform will integrate some of the most used open-source materials modelling codes (Quantum ESPRESSO and SIESTA) with models and modelling software for emerging devices (Ginestra™) via the SimPhoNy infrastructure for semantic interoperability and ontologies, powered by the AiiDA workflow engine, and its data-on-demand capabilities and apps interface (Figure 8).

Quantum ESPRESSO, SIESTA, and Ginestra™ codes are the core of the simulation engine of IM2D, and assures top-level quality solution for state-of-the-art materials modelling and advanced device simulation. AiiDA and SimPhoNy infrastructures are the foundations of the IM2D Interoperability hub that provides a standardised rich metadata set, organizing all data and information into EMMO compliant data structures. IM2D implements increasing level of interoperability: AiiDA manages the coupling-and-linking among codes and the data flux along the entire infrastructure (structural interoperability). IM2D provides a semantic level interoperability by analysing the specific use case from user, identifying what kinds of data and information need to be exchanged, and selecting the most appropriate workflows that will be operated by the simulation codes through AiiDA. IM2D upscales the existing interoperable solutions as pure Open Simulation Platforms (OSP), which are physics-independent sets of common standards and related tools that form the basic environment to develop and customize compatible and compliant simulation workflows. IM2D represents all these workflows with its own semantic based data formats. These are based on Common Universal Unified Data Structures (CUDS) that provide means to store all aspects of a workflow using a hierarchical data structure based on ontologies. In particular, IM2D the CUDS are upscaled to support the entire workflow relevant to synaptic electronics, including device modelling (see Sec 2).

An ad hoc friendly Graphical User Interface (GUI) allows to control the IM2D box, converting industrial problems into simulation cases in an easy and affordable way. It lifts the complexity related to setting up the modelling system and performing the simulation: thanks to the implemented multi-level of interoperability (i.e. structural and semantic interoperability), the complexity related to the models, pre/post-processing and data representation is completely hidden from the end user, allowing users to focus on solving the materials development problem rather getting distracted by technical details pertaining to the simulation setup. This further moves in the direction of supporting and integrating the R&D within the industrial innovation processes (see Sec. 2).

The integration of materials modelling codes and multilevel interoperable solutions makes IM2D a unique industry-driven product in the simulation software market. IM2D's value proposition can be summarized as follows:

- **To accelerate the uptake** of materials modelling software to provide industry-ready software solutions that can be taken by third parties such as commercial software companies.
- The **re-use and seamless integration** of advanced knowledge and technology, developed in academic and R&D teams, for the design of fast and easy-usable simulation solutions for industry applications (reduction of talent risk).
- **To develop core (syntactic and semantic) interoperability** based on ontology foundations and state-of-the-art software engineering standards enabling the coupling and linking of software, databases and visual interface components, and contributing to emerging standards and seamless EMMO based interoperability in MM.

- The creation of **customizable workflows** and integrated and modular simulation frameworks enabling top-down and bottom-up design of new materials, processes and devices for faster product development (time-to-market reduction).
- **To develop disruptive electronics**: demonstration of the upscaling and increased uptake of materials modelling by targeting a specific application field, namely emerging electronics and neuromorphic computing, which has a future high impact on European industry.
- The **integration** of IM2D platform and developed modules into existing and future EU infrastructures, such as the Materials Modelling Marketplace (https://emmc.info/emmc-marketplace), network of modelling translation environments, universal databases, and the Open Innovation modelling test beds.

4. Business model and marketing plan

Actually IM2D platform is in its initial development phase. At this stage any definitive or specific business model is premature. Below, we analyse the preliminary and possible business models including possible licencing solutions, funding and cost streams, and marketing plans.

4.1 Technical standards

The scientific properties and the expected advantages deriving from the distribution and the The IM2D software is in its initial development phase. At this stage the draft of any definitive or specific business model would be premature. Therefore, we only analyse the preliminary and possible business models including possible licencing solutions, funding and cost streams, and marketing plans, with no further indication of a business model we might use for the device commercialization.

The use of the proposed IM2D box has been largely discussed in the previous sections. Besides this "quality factors", the prerequisite for the release of a product (IM2D software in this case) into the market is its technical value. IM2D code implementation follows best practices of software engineering (e.g. unit testing, versioning, packaging and installation) to facilitate its future uptake and integration by commercial companies into industry ready software solutions and services. Quantum ESPRESSO, SIESTA, Ginestra^{TM}, AiiDA and SimPhoNy are already managed according to these standards. Matured experience of the implementation team assures highest standards in the realization of the software product. Specific tasks in the INTERSECT work plan (WP1.5 and WP3.5) are dedicated to put in place procedures to ensure the software is as bug-free as possible, tested on multiple platforms, easy to install and fast running. Codes and workflows will be tested and made robust and reliable before distribution. The participation in EU initiatives, such as MaX Centre of Excellence, and the collaboration with most the important computer centres, such as CINECA (IT), CSCS (CH), BSC-CNS (ES), assure the compatibility with the latest hardware developments and parallel high-performance computing.

Within the project, an aggressive action is in place to validate and test (WP3) the results generated by the software for the for important cases of synaptic electronics (e.g. OTS selectors, PCM and ferroelectric memories).

4.2 Early adopters and customers

The IM2D infrastructure is conceived for single users, companies, institutions interesting the characterization and design of advanced electronic devices, including (but not limited to) synaptic electronics and neuromorphic computing. Potential users belong to both academia and research labs and to private semiconductor industries, including fabless companies and foundries.

Early customers and strategic partnership are crucial from a business perspective. The active participation in the main decisions regarding functionalities, interactions and value-for-money needs, empower the relation with the early adopter. The first potential customers and beneficiaries of IM2D are the participant partners of the INTERSECT project. This will facilitate a future market entry. Other academic institutions, computational centres (CINECA) and European industries (IBM, STMicroelectronics, etc), active in the fields of advanced material science and nanoelectronics had already expressed interest in these products. Two members of the INTERSECT team (FRA, IMEC) are also partners of the European Semiconductor Industry Association (ESIA) [30], whose mission is the promotion of the European semiconductor industry to ensure a sustainable business environment and foster its global competitiveness.

One important action towards the distribution and commercialization is to address and empower the existing networks and create new strong partnership with the European and worldwide semiconductor industries. Establishing new partnerships and having a bunch of early adopters are instrumental for (i) shortening the time to market; (ii) reaching the most demanding customers and accessing their technology needs and (iii) keeping the development of IM2D software in line with the most state-of-the-art technologies and solutions at industry level. In addition, expanding the connections among the scientific community will also help create new synergies, compete for new funding opportunities, and investigate beyond the state of art in order to shape the future of technologies and materials.

The simple initial way to pursue these goals is to work through the established dissemination channels, such as writing of scientific papers, organizing training courses and workshops, fostering scientific collaborations, promoting the participation and exhibition at specialized conferences. Other exploitation strategies for attracting customers and maximizing the impact will be discussed in the "Business plan assessment and revision" (deliverable D4.7) due at month 30.

4.3 Position in the market and competitors

At present, there are no other tools on the market that can combine the highest levels (quantum mechanical) of materials modelling and the simulation of advanced electronic devices and memories.

This assures a privileged position of IM2D for diffusion in the semiconductor field and (in perspective) its commercialization.

Existing simulation packages for materials modelling (e.g. Quantum ESPRESSO, SIESTA, Abinit, Qbox, FLEUR, VASP, GAUSSIAN, CRYSTAL, CP2K, etc.) have been developed in academic and research groups. Despite technical differences and specific application fields, these codes provide a high-level atomistic description of the structural and electronic properties of materials on a quantum mechanical ground (mostly DFT and beyond). All these codes are not-industry-driven and generally not designed to specific application fields, thus not straightforwardly usable/appealing for engineering applications, such as nanoelectronics and memory devices. A few commercial solutions such as Biovia-Materials Studio [15], Schrödinger-Desmond [16] and Synopsys [17] offer the possibility of integrating materials modelling with high-level graphical interfaces but do not provide any functionality for device or circuit simulations. On the contrary, one of the most popular multiphysics commercial solutions, COMSOL Multiphysics [18] does not match the requirements to simulate neuromorphic devices.

In order to have a more analytic placement of our product in the market we adopted the so called SCAMPER analysis of IM2D. SCAMPER is the acronym of Substitute, Combine, Adapt/Adjust, Modify, Put to alternative use, Eliminate and Reverse/Rearrange, a mnemonic that helps to think out of the box.

• **Substitute**: Can software be swapped with another existing one?

Single engine codes (e.g. Quantum ESPRESSO or SIESTA) could be substituted by other similar codes, while the interoperable infrastructure has no similar alternatives.

• **Combine**: Is it possible to combine present software with another one and create something new?

This is one of the strength characteristics of IM2D, which integrates and uptake existing state-of-the-art models and codes. The modular structure of the infrastructure allows to further extend IM2D to other models (e.g. mesoscopic entity) and other codes (e.g. classical molecular dynamics).

• **Adapt/Adjust**: Can this software serve other purposes beside the one intended? Can the software be adapted to serve non-expert users?

The synergic combination of material and device modelling can enable the application of the IM2D interoperable solutions to several industrial fields, even beyond synaptic electronics. A few examples include: artificial intelligence and machine learning, sensors and bio-sensors for, e.g., building, heritage conservation and medical analysis, batteries production, photovoltaics, fuels cells, energy storage devices; power devices and actuators.

The semantic level of interoperability is explicitly conceived to reduce the complexity of the physical problems, getting access to material-to-device modelling also to non-experts in the field.

• **Modify**: What can be emphasised in the software to create more value? Is it possible to modify an element within the software to create something new?

Materials discovery and characterization of material properties “on demand” are among the declared capability of the software. At present, no other available software product can integrate the existing know-how on material science and the advanced characterization of the emerging memory device as IM2D.

• **Put to alternative use**: Could another industry/domain profit from this software?

The interoperable solutions developed within the project can be further exploited for the release of stand-alone apps for high-level customized solutions (e.g. metadata and GUI management).

• **Eliminate**: Less is more – is it possible to simplify/streamline the software tool? If easier, would it be more attractive to users?

The development of the IM2D is at its early stage. Optimization and simplifications are important points that we consider in the validation and internal evaluation of the software. More actions on these aspects will be assumed when the IM2D is more consolidated.

• **Reverse/Rearrange**: Is it possible to rearrange the workflow you offer?

The implementation of semantic interoperability as OSP will allow us to customize, rearrange workflows, as well as to manage and write new ones, depending on the offer.

This simple analysis confirms the strength and the potential value of IM2D in the semiconductor and materials modelling markets. The combination of device level simulation (Ginestra^{TM}) with material modelling (Quantum ESPRESSO, SIESTA) will tremendously increase the application of IM2D software in the area of emerging nanoelectronics devices for neuromorphic computing and artificial intelligence, where a new bunch of materials (currently not addressable by device modellers) can be eventually investigated.

4.4 Market plan

The Market plan is under construction. At this development stage, the partners of the INTERSECT project and the AEB are drafting and planning the exploitation and dissemination strategy. A list of business-related KPIs and a first communication plan have been already defined (Deliverable D5.1 “First report on project’s governing bodies, KPIs, and setting up”, month 6).

4.5 Exploitation Strategy

4.5.1 Exploitation of knowledge

One of the main commercial values of the INTERSECT project is its know-how. Within the project the intellectual property (IP) management is carried out by the Project Coordinator and the Governing Board. Other ad hoc entities (not yet identified) will be necessary for the steps beyond the project. The potential IP asset (software and/or technology) will be evaluated in terms of technology relevance, potential applications on the relevant markets ('technology pull'), and the ability to progress the technology or solution beyond the state of art. Specific IP regulations will be undertaken with industrial advisors under *ad hoc* non-disclosure agreements.

4.5.2 Exploitation of IM2D infrastructure

IM2D is expected to become a unique simulation product that, by best exploiting advanced software and interoperability infrastructures, will enable to increase the simulation role in the design of novel devices (i.e. neuromorphic systems) that the stand-alone models today are not able to tackle. The exploitation strategy is still under development, but what is clear is that IM2D will directly contribute to European cloud services and Open Science Platforms via integration with the MarketPlace project. This will enable new strategic partnerships, building trust on modelling activities and create new university-industry relationships. The entire infrastructure can be re-deployed completely or in part inside the firewall of a company, or on the cloud, thanks to the containerization and virtualization solutions already adopted in the Materials Cloud [31].

The potential enhancements of the interoperability level in terms of efficiency, flexibility and optionality of combinations of semantic ontology-based tools and data curation for the domain of INTERSECT is completely untapped. Fully interoperable, ontology-based wrappers and orchestrators in the OSP sense have not yet been integrated in professional software tools in this domain. On the basis of the market requests, we are open to the different possible commercialization routes which consider, for instance, the commercialization of the overall IM2D platform or of stand-alone interoperable modules for high level custom solutions, such as general apps for metadata and GUI management or interoperability modules for the interconnection among the stand alone codes considered in the project.

Details and regulations have not yet been defined and will be the subject of the second Business plan ("Business plan assessment and revision", deliverable D4.7, month 30).

4.6 Ownership and Licensing

Most of the codes gathered in IM2D (QuantumESPRESSO, SIESTA, AiiDA, SimPhoNy) have been developed in academic research groups and are open source codes. As such, the IP management is substantially simplified: all codes, documentation, and project information are freely available under GPL licence and reusable for any potential use, be it commercial or not. At odd, Ginestra™ is a commercial code distributed under a proprietary license. All newly released libraries and modules developed within INTERSECT as well as the IM2D interface will be licensed in such a way to be compatible with usage by third party codes, including commercial ones (e.g. using LGPL or MIT-BSD license). This will reinforce the European open-source ecosystem and fulfil the mission of most of the academic partners towards open software and open data production.

The project goal is the realization of a "pre-competitive" software solution that will provide the natural basis for start-up creation beyond the project end. This will allow the members of the consortium to create and develop their own commercial product. Furthermore, both the "pre-competitive" and "competitive" interoperability layers will share the same interfaces (e.g., API) which will allow third parties to develop their own compatible solutions so to increase the ecosystem of interoperability (e.g., replacing part of the codes with others).

More specific aspects about ownership, legal partner agreements and licensing forms – too premature at this development stage – will be discussed in the next deliverable "Business plan assessment and revision" (D4.7, month 30).

4.7 Data and confidentiality

It is expected that the research data produced within the project will be made findable, accessible, interoperable and reusable (FAIR). This, however, does not imply any obligation by project partners or other external users to share their own data or make them public beyond this project. The Materials Cloud dissemination platform provides the most comprehensive capability in this respect for calculations and data in computational science.

Leveraging the multi-level interoperability modules allows us to go significantly beyond current standards and the state-of-the-art in the field, by storing not only the results of calculations, but automatically recording their entire full provenance with rich metadata in a standardised format and convertible to other formats with dictionaries. In particular, the open data dissemination platform Materials Cloud [31] allows to expose to the community at large raw data (Materials Cloud Archive), curated data (Materials Cloud Discover), and full calculation workflows (Materials Cloud Explore); these can be automatically uploaded when using the AiiDA infrastructure and only if the users willingly upload their AiiDA databases to the Materials Cloud.

In the interaction with industrial users it usually necessary to provide confidentiality for either the specific simulation of interest, the data resulting or specific development activities that may be time or market sensitive. In this case, it is expected that for industrial users and consultants generated data would remain, at least initially, within the company firewalls. Data documentation is independent from user's distribution policies: both open and confidential data will be produced, traced and curated with the same standards. Furthermore, IM2D shall use an internal registry of all data exchanged between partners or produced, especially on confidential data and either open or proprietary data with potential for exploitation.

Further details on generation, curation and storage of data are available in the INTERSECT "First data management plan" (Deliverable D4.2, month 6).

4.8 Revenue and cost streams

A detailed revenue and cost plan is under construction: important variables - such as licence, IP, personnel, etc., necessary for an actual commercialization plan - are still under discussion. These factors will depend not only on the commercialization intentions of the proposing partners, but also on the specific market requests at the commercialization time.

Some of the possible revenue models considered for IM2D are: (i) mixed open-source/commercial business model, (ii) services and consulting, (iii) government funding. The mixed open-source/commercial model conjugates open source business model and code sale and maintenance service, through subscription of software licensing, (today only for the proprietary part of the infrastructures Ginestra™). This business model is based on the partnership between academic institutions and commercial software vendors. In Open-source based business models, the main value comes from key people's knowledge and expertise. These assets are relevant for SOW of Quantum ESPRESSO, SIESTA, AiiDA and SimPhoNy, softwares that have been developed by high-skilled scientists and distributed in free versions under GPL licenses. The business model of open-source business is to offer consultancy and solve customers' problems through code development and maintenance. Revenue is based not only on services, but also on 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. This overlaps with the Services and consulting model, with services that range from very limited services of maintenance to more extensive implementation, customisation, training, technical support or consulting, and contract research services. Government and public funding models turn out to be essential in the case of development of open-source software or major upgrade operations: it can take 10 or more years to develop a materials modelling code and make it mature and ready for industrial applications. Open-source codes in IM2D have been completely developed in the last decades on the basis of government or public fundings, such as national and European project grants (such as INTERSECT). Only Ginestra™, is a commercial materials-device simulation software owned by Applied Materials, www.appliedmaterials.com/mdlx.

Revenues and costs can be classified in terms of the economic elements corresponding to their "nature" or "destination" as shown in Table I below. The articulated list of the costs requires careful attention and a dedicated management structure. In INTERSECT the management structure reflects the project governing bodies. The Advisory and Exploitation board leads the business-oriented activities designing the dissemination and exploitation strategies, monitoring the engagement activities, and managing the generated innovation and IP related issues of the project.

CRITERION	REVENUES	COSTS
by "nature"	-Consulting -Code development -Training -Other activities	-Management activities -Marketing activities
By "destination"	-Provisions of services -Contribution for projects financed externally by national or EU public entities -Membership fees -Contributions in-kind for	-Personnel costs (including developers, researchers, technicians, and administrative) -Cost for technical-scientific services provided by members -Costs related to funded activities

	resources made available by members	-Costs related to internal projects (funded by members with membership fees) -Costs related to resources in-kind by members -Costs for services provided by third-parties -Armonization/deprecation -Other general expenses -Financial charges -Legal costs -Taxes

Table I. Classification criteria of economic elements

As aforementioned, a detailed plan for costs and sustainability of the IM2D software is considered premature and not conclusive at this stage of the project and of the software development and thus we postpone it to the “Business plan assessment and revision” (deliverable D4.7), due at month 30.

4.9 Business Model Canvas

A summary of the preliminary IM2D business model is displayed in Figure 11.

KEY PARTNERS	KEY ACTIVITIES	VALUE PROPOSITIONS	Stakeholder RELATIONSHIP	Stakeholder target SEGMENT
EMMC Council Network European Semiconductor Industry Association (ESIA) members Computational centers (CINECA) EU semiconductor industries(IBM, STM,..) EMMC Marketplace Members	Development of IM2D platform → multi-physics, multi-model, multi-equation, hierarchical and scale-reversible model for material-to-device and device-to-material optimization for an easier exploration of the material workspace from an electronic device-oriented industrial perspective	IM2D will solve these critical aspects: **QUALITATIVE** -More efficient and targeted exploration -Reducing of screening by experiment (cost, time) -Minimization of lab tests -Deeper Understanding of quantum mechanical electronic and atomistic phenomena -Reducing of lack of acceptance of quantum mechanical electronic and atomistic models -R&D strategy development -Enhance troubleshooting avoiding dead ends of experiments -Accurate device/ nanostructured materials analysis and optimization **QUANTITIATIVE** -IP generation -Cost saving by cutting development time and saving of experiments	-Co-creation of the solution -Creation/Contribution to scientific communities.	-EDA (Electronic Design Software) and more specifically of the Technology-CAD (TCAD) -EU Semiconductor industries -Scientific & Professional Communities
	KEY RESOURCES -IM2D will be an integrated and interdisciplinary tool which encompasses: -SimPhoNy, a Simulation framework for multi-scale phenomena in micro- and nanosystems -AiiDA, an Automated Interactive Infrastructure and Database for Computational Science -Quantum ESPRESSO (QE), a suite for quantum mechanical modelling of solids, interfaces and nanostructures. -SIESTA™, a general purpose DFT code based in the use of confined, numerical atomic orbital bases, and designed for efficiency and computational speed. -Ginestra™, a commercial software designed to simulate the electrical characterization measurements performed on semiconductor devices for an easy interpretation of the experimental data and for the prediction of device reliability.		**CHANNELS** Dissemination: -Open access publications -Social media activity -Website -Presenting in key -Conferences (IEDM) -Tradeshow -Infiltrate actions into forums and blogs	
COST STRUCTURE Personnel Travels Dissemination costs (Open Access and Conference/Tradeshow Fees)		**REVENUE STREAM (prospects)** New Strategical Partnership		

Figure 11 Business Model Canvas

Acronyms

ADAS – Advanced Driver Assistance Systems
AEB - Advisory and Exploitation Board
AI – Artificial Intelligence
BDSS - Business Decision Support System
CAE - Computer-Aided Engineering
CAGR - Compound Annual Growth Rate
CUDS - Common Universal Unified Data Structures
D&A - Data and Analysis
DRAM - Dynamic Random Access Memory
EMEA - Europe, Middle East, and Africa
EMMC - European Materials Modelling Council
EMMO - European Materials Modelling Ontology
FeRAM - Ferroelectric RAM
GPL - GNU General Public License
GUI - Graphical User Interface
IM2D – Interoperable material-to-device
IoT – Internet of Thing
IP - Intellectual property
KPI - Key Performance Indicator
M&A - Merger and Acquisition
MM - Materials Modelling
OSD - Optoelectronic, sensor and discrete components
OSP - Open Simulation Platforms
PCM - Phase Change Memory
R&D - Research and Development
RoI - Return on Investment
SaaS - Software as a Service
SSD – Solid State Drive
SWO - Software Owners

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