EMMC-CSA

European Materials Modelling Council

Report

on

"Story boards of materials modelling"

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The workshops and the preparation of the reports have received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement No 723867

1. Executive summary

1.1 Description of the deliverable content and objectives

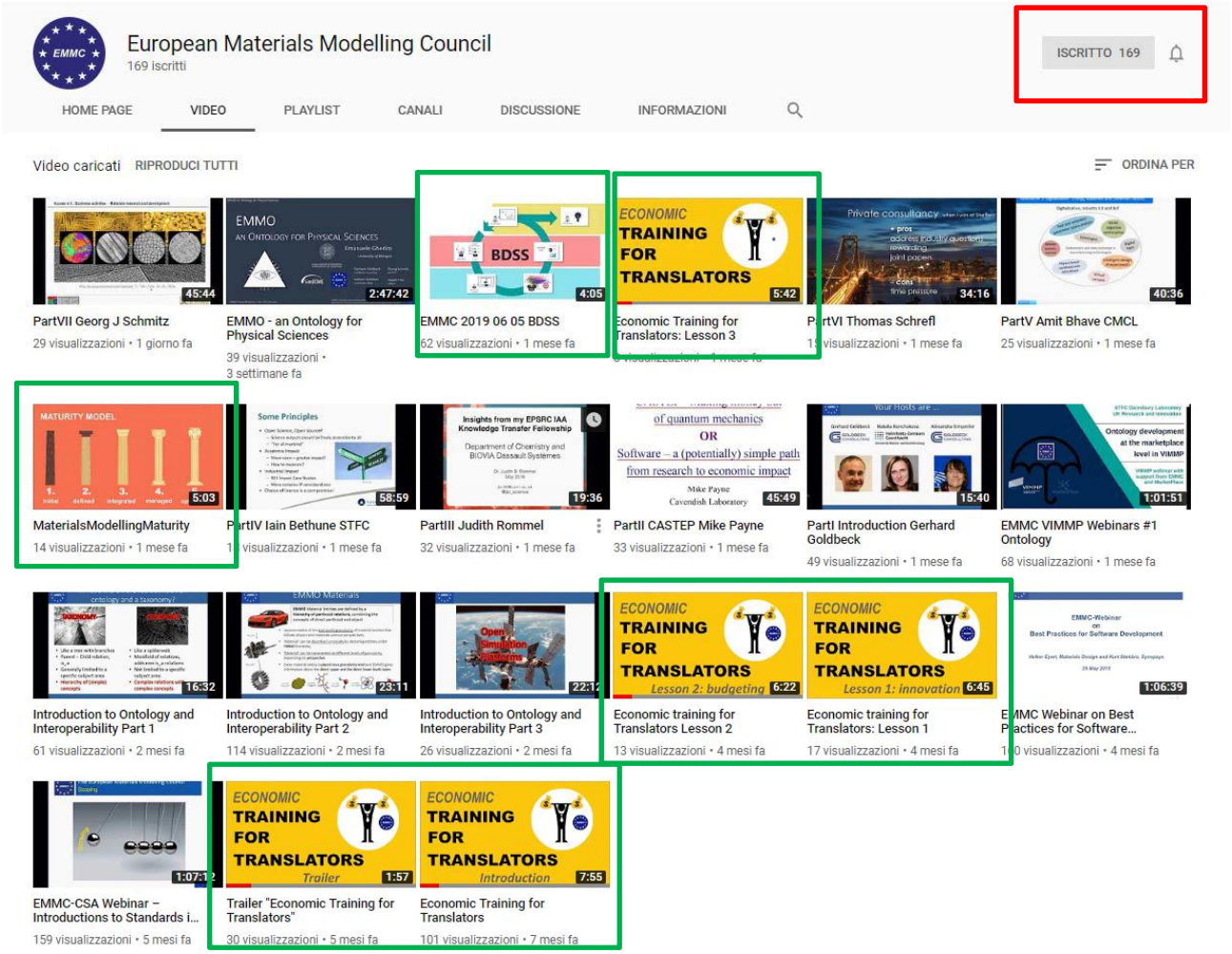
Several storyboards have been developed for the video series on the economic training for Translators, Maturity model, the Business Decision Support System (BDSS) and EMMC Case Studies. The reported storyboards particularly refer to Task "Enhance the visibility of materials modelling possibilities to industry, in particular SMEs" of the EMMC-CSA working programme.

1.2 Major outcome

The major outcome is a series of 6 videos, whereby the first 4 are related to economic training concepts for Translators and two additional ones relate to the Maturity model and BDSS. All the videos are publicly available on the EMMC YouTube channel

https://www.youtube.com/c/european-materials-modelling-council

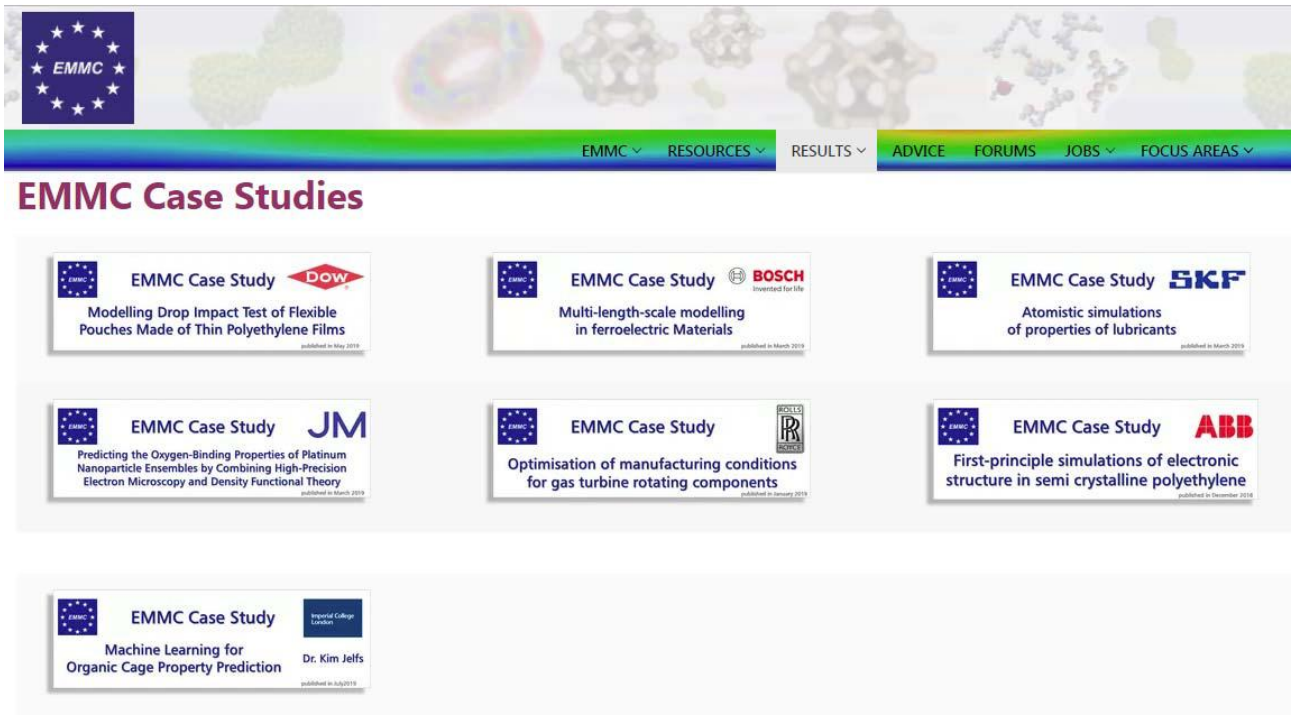
Below is a screenshot of the EMMC YouTube channel with the available videos



The number of subscribers to the EMMC YouTube channel is 171, which is a quite consistent number of users, most of them from the EMMC community (invited to subscribe via the EMMC contact list).

In addition, the BDSS video has been showed during the EMMC International Workshop 2019 inVienna, during the session organized by the Working Group "Industrial Integration and Economic Impact" dedicated to BDSS systems.

The story board of Case Studies (https://emmc.info/emmc-case-studies/) is presented below:



Each of these "stories" can be accessed by clicking their banners and the story is accessible online or a .pdf file can be downloaded. We covered modelling performed by industry, by 3rd parties, and databased materials modelling performed in academia. Each story was reported on twitter and LinkedIn and we could find several 100ds of interactions worldwide.

2. Progress report (main activities)

2.1 Video 1: Introduction video

The introduction video was developed to introduce the videos series about economic training concepts for Translators. A "Full" version was developed together with a "Short" version trailer extracted from the main video, meant to be used for distribution on EMMC social network to refer to the full video on the EMMC channel. Both videos are publicly available on the EMMC YouTube channel.

The story board is reported below.

Today a lot of Companies try to innovate, to find innovative solutions for their business problems.

Let us take a look at some business cases:

- *Alpha is a SME which main application sector is Defense and Energy. Alpha wants to know more about the tensional and microstructural state of gears, to determine the origin of distortions, which causes rejected components;*
- *Then we have Beta, a large enterprise involved in organic electronic materials and devices.*

But for both Alpha and Beta these innovations seemed impossible to achieve.
What were the reasons? Let's try to build a logical path.

First of all, what "Innovation" really means? Innovation is not doing something new or something better. We start from DISCOVERY to discover something new that generates ABSTRACT KNOWLEDGE; Then we move to the INVENTION makes that abstract knowledge able to SOLVE A PROBLEM, and finally we arrive to
INNOVATION when that discovery has an UTILITY for someone and is able to generate an ECONOMIC RETURN.

Now, what about research process?

First steps of the road to innovation take place in UNIVERSITY. University research is not constrained by market needs; therefore, scientists are free to experiment, fail and try again. But what is the difference between research in University and Company?

- *Company Research:*
  - *Specific for its contents*
  - *The aim is to go to the market*

But firms have some problems:

- *Lack of qualified human capital*
- *no time and budget for numerous trials & error*
- *market deadline - not allowed to do big mistakes*
-

While University Research:

- *various areas of competence and qualified human resources*
- *large quantity of specific tools from different departments*
- *always up-to-date research*

So, without university, there is no quality and updated research and without firms, ideas not become innovations.

But in reality, University and Companies do not cooperate efficiently. Why? They are two distant worlds not only for different ways of acting, visions or goals, but most of all, for a different language used. Academic language is often too abstract and technical for more concrete business realities.

An area that particularly requires innovation is Material Modeling. A model is a mathematical representation of a system, in this case a material, to be solved numerically through simulation programs. MATERIAL MODELING is a highly technical field that requires experienced personnel, with strong physical and chemical knowledge, and ability to manage relative software, but often these technicians are not present in companies and therefore university studies are not understandable by companies.

Alpha and Beta had exactly these problems: they must do a lot of trial & error experiments, which are very time and cost consuming; this can be solved by using simulation software, but the competences and knowledge in these companies, both in technical terms and in software usage, were not sufficient to face up to these innovative issues. So, how can Alpha, Beta and all the other companies solve these problems?

It is important to underline that a company cannot simply acquire competences from the outside: We must consider that each company has its ABSORBITIVE CAPACITY, the ability to recognize the value of new information, assimilate it, and apply it to commercial ends. And ability to learning is also determined by the characteristics of the knowledge: the more complex it is, the more difficult will be to integrate it.
So, it is necessary a figure who has skills from the academic world and who can apply them to concrete business cases, to assess the feasibility and convenience of innovation, through the use of a common language; Then a new figure is created: The Translator, which "translates" practical request from companies into modelling activities (also for academia), guiding companies towards the understanding of innovation.

Who is the Translator? A figure who must possess both a technical and economic background, combined with various soft skills, to be able to make strategic decisions for the company.

The translator can be of different types:

- *Academic: Comes directly from the University reality, with a strong technical and scientific expertise, often with previous research experiences*
- *Internal: Working in large companies as an internal translator that incorporates his specific knowledge to the company, able to reduce problem solving time and creating a closer contact with customers*
- *Independent: In SME as an external consultant, as a software and technic expert, helps small realities which often have little time, resources and budget for research and cannot afford an internal Translator*
- *Software Service Expert: Comes from a Software Service Company and works as an external consultant, both for large and small companies, and besides having important skills in the use of simulation software, he is also the owner.*

Each company, based on its type of project and its absorbing capacity, can therefore have its perfect Translator, which will be able to transform an engineering problem into a modelling/computational problem, and bring it back, resolved, to the corporate reality.

How does the translator bring value to the company? Through the use of tools for modeling and simulation, interpreting the data obtained, is able to find the best solution for the business problem and evaluate its economic and technical feasibility, reducing the number of experiments and the necessary study, thus saving time and, consequently, cost.

The "Training for Translators" program aims to provide all the economic / managerial knowledge necessary for the training of this professional figure, which will be added to their previous technical skills and ability of using specific modeling software.
Video lessons about economic knowledge and related topics will be provided by EMMC, in particular:

- *Concepts about economic & management of innovation, business management;*
- *project management, planning knowledge and communication skills;*
- *intellectual property*

2.2 Video 2: Innovation

The storyboard for the second video about innovation is reported next.

INNOVATION COURSE

I am Francesca Montagna, I am professor at Politecnico di Torino of Innovation Management and New Product Development; I am an industrial engineer. Now my research topic mainly concerns the dynamics of innovation and the management of new product development processes, with a particular focus on the design decisions and the method to support design decisions.

This course will concern topics like innovation management and new product development. This kind of topics are important for Translators because Translators have ***to learn what innovation actually is*** *and have to understand how to manage these kinds of innovation, and how the strategies for innovation can be developed. Moreover, it will concern also the new product development process and the* ***competences that are required in the management of the new product development process.***

Differently from what people think, innovation is not something new, but before having a product an innovation, we should have this product adopted. So, the adoption is a condition that is necessary to have an innovation, well instead novelty is a requirement, but it is not sufficient. The dynamics of adoption and the dynamics of innovation are therefore relevant to understand how to make a product adopted and how to make a product an innovation. We should understand together

the differences between radical innovation and incremental innovation, and the real meanings of these terms, that does not mean necessarily little innovation or big innovation.

The Translator therefore, must understand the innovation dynamics, what is a paradigm, the emergence of a new paradigm and how, eventually, dislodge the past paradigm.

Studying innovation therefore means also understanding how to manage innovation and how to define a strategy for innovation. Usually, a strategy for innovation concerns the understanding of the project portfolio, the competences that the company has and the competitive environment in which the company works.

When we consider an innovation contest, the competitive advantage is not stable, but it is temporary, and the sustainability of the competitive advantage is obtained just identifying the right strategy. We try to understand which are the possibilities that the company has in order to define the right strategic roadmap.

An innovation strategy is made of new competences that must be built and is made also of an organizational process that is the organizational learning. Companies evolve by learning and hence the Translator has to know how the company learn. Two possible process of learning exists: we have exploration processes, when companies try to understand new possibilities of business, try to find new solutions, try to understand new alternatives, but **this kind of processes are far from the competences the companies already have.** *Well instead, we have another process that is the exploitation process of learning, by which company learn by doing. So, from the operation processes, the day by day processes,* **the company learn how to do things and evolve by doing things.**

So, the translator must know this kind of processes in order to understand how competences can be gathered in an organization.
The evolution of a company depends on learning but also depends on the ability that each company has to absorb these competences; this is usually named **absorptive capacity.**

Gatekeepers are figures that are relevant for acquiring the right competences and for absorbing these competences inside the company. This is because this kind of figures have technical competences so they are able to understand what is the right competences to be acquired, but they also have a communication role, a recognized role inside the company and consequently they are able to transfer what is gathered from outside the firm, inside the firm.

Translators are really similar to gatekeepers *because they have technical competences, so it is likely that their role in companies will become similar to the one of gatekeepers.*

Finally, the course will focus on new product development, the organizational process in which innovation occurs. The translators have to know the dynamics of the new product development process, the activities inside and the variables that are relevant for its management. This is because **Translators can work like a bridge between the technical part of a company and the management one.**

So that, the design decision can be comprehended also in term of impact they have on the operation and management processes, and on the other side managers can understand and explore the innovation possibility, also with respect to the design capability and the technical competences inside the company.

2.3 Video 3: Capital budgeting

The storyboard for the third video about Capital Budgeting is reported next.

In this course we will discuss how managers take decisions in long term and how can they use money in order to make investments. So, the issue is that managers ask for some budget and they decide which investment is more profitable for the companies where they operate. Capital budgeting is important for translators because they will complement the technical knowledge with an economic knowledge and in this way, they will be able to understand language of managers and the reason why they make investment in companies.

Part 1. We will understand that an investment is the usage of monetary resource that is expected to produce a future return of the investment.

Part 2. Some example of an investment in a company can be the introduction of a new product, so company can decide if including in the portfolio the production of the new product, or they can extend the facility. In this way, the ***translator will be able to understand the NET PRESENT VALUE (NPV)***

Part 1. In the evaluation of an investment, company can decide to use some different methods. The methods most used by companies is what is called the NET PRESENT VALUE. Company when decides to make an investment has to consider two main cash flows: the first one is the initial investment, that is the amount that the company use when they made investment in time 0; time 0 is the time when managers decide to make an investment. The second component that is used is the series of cash flows that occur in different periods according to the years and economic life of an investments.

Part 2. Because Net Present Value is the sum of different cash flows that occur in different periods, it is not possible to directly sum all these components. This is the reason why we will discuss about discount rate; we will learn what a discount rate is and how we have to compute the net present value. When we find the NPV more than 0 it means that the return of the investment is higher than the required return of an investment. And we will learn what means that the NPV is equals to 0 or less than 0.

1. *Discount Rate*
   Part 1. Usually company use discount rate as cost of capital. The cost of capital used in evaluating the NPV is even by two main components: there is the cost of debt capital and the cost of equity capital; they are sum by weighting each component by the weight of the debt and of the equity over the total capital structure of a company.
   Part 2. Evaluate the cost of capital will be quite simple, for evaluate the cost of equity capital will be difficult because shareholders have to consider the opportunity cost of using the same money for alternative choices.
2. *Cash Flow*
   As said before, we will compute the value of the NPV by considering the cash flows that characterized every period of an investment. We will learn during this course which are the different costs to consider in the evaluation of an investment, what a sunk cost is and also what an opportunity cost is and how they impact in the evaluation of the investment considered by managers.
3. *Other methods*
   Part 1. In the last part of the course we will discuss alternative methods for evaluating an investment. For example, we will have a look to other two main methods: the first one is the payback period and the second one is internal return rate.
   Part 2. Payback Period represents the number of periods that are necessary to recover the investment.
   Part 3. We will be careful that NPV is not a measure of profitability of an investment but of liquidity; so, we will learn how the NPV and the Payback Period can be different and the reason behind their choice in the company.
   Part 4. Internal Rate of Return (IRR) is the rate that equals NPV to 0. It means that IRR represents the rate of return of the funds of the project of the company.
4. *Conclusion*
   To sum up, this course "capital budgeting" ***will be able to provide the method for evaluating an investment.***

Video 4: Intellectual property

The storyboard for the fourth video about Intellectual property is reported next.

INTELLECTUAL PROPERTY RIGHTS (6M-6M30S)

1. Brief introduction (20-25s)
My name is Antonio De Marco, I am Assistant Professor at the Department of Management and Production Engineering of Politecnico di Torino. My research is in the area of the economics of innovation and intellectual property, with a specific focus on patent data, markets for technology, and technical standards.
2. Motivation (80-90s)

*In this course, translators will learn the basics of intellectual property rights. **Why is intellectual property relevant when it comes to innovation management?** Well, let me start with some stylized facts. First, let us have a look at the companies that in the seventies were in the Fortune 500 list, the largest corporations in the United States: for those firms more than 80% of the market value derived from tangible assets (that is machinery, buildings, land, and so on) while only about 20% of their value came from the so-called intangible assets. Now, let us look again at the Fortune 500 list as it is today. The previous statistic would be reversed: 85% of company value is now associated to intangible assets mostly deriving from investment in innovation. This evidence shows that firm competitiveness is strictly connected to continuous innovation and to the acquisition of the competences and capabilities for managing innovation activities in the most effective way. Second, it also shows that competitive intelligence should pay extra attention to the sources of information on innovative activities.*

3. What are intellectual property rights? (120-130s)
*Intellectual property rights include patents, trademarks, and copyrights. In the course we will specifically focus on patents. The basic idea is that if you have invented a new product, a new process, or, more in general, a new technical solution to a problem then you can file a patent application and **ask for protection from imitation**. As a patent owner you will have an exclusive right to prevent and stop others from commercially exploiting the patented invention or from patenting similar inventions. These property rights allow the holder to exercise a monopoly, but the social costs of monopoly power may be offset by the social benefits of higher levels of creative activity. In exchange for that, the inventor should disclose technical information about the invention that normally becomes public after 18 months. Patent rights are also territorial rights meaning that those exclusive rights are only valid in the country where the patent has been (previously) filed. The protection is granted for a limited period, it generally lasts 20 years starting from the application date.*
The number of patent applications that are filed globally is constantly increasing (chart 1). In 2016, 3.1 million patent applications were filed worldwide (that is an 8% increase with respect to the previous year). 40% of those patent applications were filed at Chinese patent office (chart 1A). Finally, just five offices (China, the USPTO, Japan, Korea, the EPO) received more than 80% of all patent filings worldwide. Each country is specialized in different technological fields (chart 2).

4. Why patents are useful for firms? (140-150s)
*Patents are an essential tool for firms for several reasons. First, having a strong portfolio of patents is crucial in order to achieve success in legal actions against those who copy the protected invention. Second, a high-quality patent portfolio can be seen by investors, customers, and other stakeholders as a signal of the technological capabilities and specialization of the company. Third, **since patents can be sold or licensed to other firms, they can facilitate technology transfer among companies.***
Finally, there is an additional way of using patent data. It is well known that about 80% of the information disclosed in patent documents cannot be found in other sources. In most of the industries, patents are a valuable source of information supporting management decisions. Firms can ascertain if their new inventions meet the requirements for patentability and the extent of their freedom-to-operate (i.e. they can avoid infringing the patents of other companies and discover potentially blocking patents); firms can monitor the innovation activities by understanding the key innovation trends and identifying the key players and their IPR-related strategies; they can discover potential R&D partners, licensees or licensors; they can use quantitative data from patent documents to support the evaluation of R&D projects and other business decisions.

*The use of IPR can be tailored to different needs according to firm size. Not surprisingly, an effective management of **patent rights is not only beneficial to large corporations**. In fact, intangibles are embedded into every business, even those of small companies. Translators need to properly understand the specificities of the firm, the goals set by the stakeholders or users that belong to the management or to the technical areas of the company.*

Video 5: Maturity model

The storyboard for the fifth video about the Maturity Model is reported next.

WHAT IS MATURITY MODEL

Companies often operate in their business without being aware of their strengths and weaknesses: acquire awareness of their own situation can allow them to set their goals and make them real.

Some tools can be used to help this; in the field of Materials Modeling the Maturity Model has been developed: by analyzing the current situation, this tool allows to create a map of the "as is" and "to be" situations, to understand how to reach the goals and improve the performance.
In the context of Materials Modeling, a corporate structure can be thought of as consisting of four fundamental pillars: people, processes, date, tools. Each of these pillars can be found at a different "maturity" level. In order to grow and succeed, a company must be able to improve in all these four sectors, by moving from one level to another; companies thanks to the maturity model can understand at what level of maturity their pillars are and understand at a what level they want to bring them.
However, companies are often blocked by some barriers in the transition from one maturity level to another; how can barriers be defined? A barrier is something like a rule, a law or a policy that makes it difficult or impossible for something to happen or be achieved. Or, from another point of view, prevents two people or groups from agreeing, communicating or working with one another.

They concern all the four pillars and can be defined as:

- *technical barriers (non-integrated tools, usability and functionality of tools);*
- *communicative barriers (communication problems between different company departments, lack of required skills, non-communication between modelers and non-modelers, different intra-company objectives);*
- *and economic barriers (not enough budgets, low investments because the importance of these topics is often not understood).*

This is often due to the fact that many times companies fail to understand their situation and, therefore, fail to realize what are their real problems that prevent the transition to a higher level of maturity and, so to the business' growth.

The maturity model makes it possible to understand where a company is starting from and, therefore, to start laying the foundations of an improvement: The awareness of where a company is and where it wants to arrive is the key point for its success.

The proposed model considers five levels of maturity: initial, defined, integrated, managed, optimized; these levels concern each of the pillars. For example, if you are at the initial level for the "process" pillar, your processes would probably be based on individual skill and choice and therefore they would be highly variable; while, at the optimized level, the processes would be well documented and accessible, fully integrated in business decision and consistently deployed.

A lower level of maturity often leads to unpredictability and inconsistency, which will decrease and instead find more and more advantages as you become more mature. An optimized level allows timely and reliable in-depth analysis and integrated, informed and dynamic decision-making processes throughout the organization.

HOW DOES IT WORK

So, if we imagine that you are one of these companies in the field of material modeling… how do you figure out where you are? You will be provided with a questionnaire structured in this way:

For every pillar are presented 7-8 questions to which you can answer by selecting a score from 1 to 5, which represent the increasing level of maturity: two sentences are provided that clarify the meaning of the score 1, the initial level, and of the score 5, the optimized level.

For each question, you have to respond by selecting the score two different times, as you should give information about two distinct scenarios:

1. the current situation;
2. the target situation where you want to arrive in three years

For every pillar, at the end of the questions there will be a self-assessment, where you have to answer a generic question by selecting one of the five possible sentences.

Through the analysis of these data, it is possible to understand how your corporate structure is constituted:

- *by observing the general average: this is the basic idea of how the company is structured;*
- *by comparing each pillar with the average: one can understand whether there are areas more or less mature than the general corporate level;*
- *by analyzing the individual areas*

This can lead, for example, to understand that you have a company that seems very solid but has strong lack in a single area, or vice versa can help you understand what your strengths are.

The practical output that you get is a radar chart that indicates the current and target level of corporate maturity: the closer you are to the center, the more you are at basic maturity levels; the further away you go, the more you are at an optimized level.

2.4 Video 6: Business Decision support system

The storyboard for the sixth video about the Maturity Model is reported next.

Materials modelling, from electrons and atoms to macro-systems, is a key strength of the European Science & Technology community.
To fully exploit the value of materials modelling, a deeper integration within business decision-making processes is essential.
Industry uses information systems, sometimes known as Business Decision Support Systems, or BDSS, to enable faster decision making and better allocation of resources across the business.
BDSS which integrate materials modelling enable the following well-established benefits:

- *R&D strategy development*
- *Improved functionality for performance-driven materials such as weight reduction*
- *More efficient, reduced experiments*
- *Grow and secure Intellectual Property claims*
-

To realize these benefits, successful business decisions rely on complex information condensed by Key Performance Indicators or KPIs. KPIs, can be used to measure performance of projects, departments, individual sites, organizations, and across the supply chain.
Typical KPIs could be:
- minimizing production costs
- maximizing product strength
- meeting regulatory targets
KPIs can draw on information from multiple sources.

Traditionally, materials information comes from expensive experimentation. Today, materials modelling can deliver information rapidly, and accurately offering providing precise, actionable intelligence.
Materials modelling enhanced BDSS can quickly provide knowledge for informed business decision-making, empowering:

· *Seamless integration within existing company structures*
· *The ability to combine materials models with disparate information sources including economics, supply chain, market trends, pricing, and customer requirements.*
· *The selection of appropriate material models for the application, whether a material, product, or manufacturing process*

· *Accelerated decision-making*

- *New insights and knowledge to drive business performance*
- *Enhanced predictive power of product life cycle management systems*

Despite all the advantages, currently no commercial materials modelling incorporated BDSS exists. The European Commission is aiming to put forward rational design principles to develop prototypes of such systems as the basis of future commercialization, incorporating:

- *COMPOSELECTOR focusing on composite materials*
- *And FORCE focusing on chemical formulations*

Although tackling challenges in different material domains, the projects converge on the definition of how to integrate materials modelling in Business Decisions Support Systems.

Materials modelling, business tools and databases integrated into a framework empowers decision-makers at all levels of the business.

- *At the strategic level, the VP/Product Engineer or Scientist will define the business KPIs: for example, minimizing cost or risk or improving product performance*
- *At the tactical level, the senior manager will translate the KPIs into model & simulation workflows and define Model KPIs: for example, maximizing accuracy of models or minimizing computational costs. This step could be further supported by external experts.*
- *At the Operational level, the material engineer or scientist will perform the simulations and feed-back the simulation results and the model KPIs*
- *The validated business KPIs for different scenarios are summarized in the form of charts or graphs, hiding the complexity of the simulation data*
- *These KPIs enable informed, strategic business decisions*

Materials modelling has the potential to transform the way we make decisions as engineers and scientists …

2.5 Case Studies

2.5.1 ABB Case "First-principle simulations of electronic structure in semi crystalline polyethylene"

The case is based on ABB's work in studying electrical insulation materials and their publication, which was a joint effort with KTH,

"First-principle simulations of electronic structure in semi crystalline polyethylene", A. Moyassari, M. Unge, M. S. Hedenqvist, U. W. Gedde, and F. Nilsson; J.
Chem. Phys. 146 (2017) 204901 (DOI: 10.1063/1.4983650)

2.5.2 Rolls-Royce Case: "Optimization of manufacturing conditions for gas turbine rotating components"

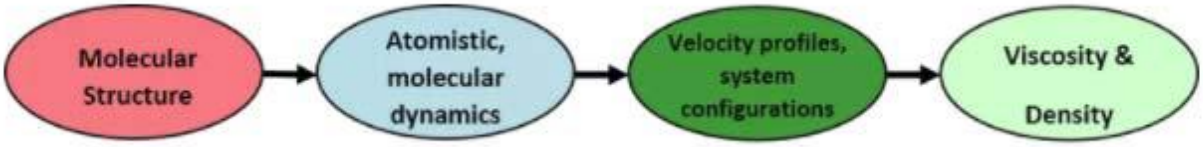
The case study is based on a project between Rolls-Royce and the University of Birmingham, "The development and application of a mean field precipitation kinetics model to the optimization of manufacturing conditions for gas turbine rotating components", which was presented at the 1st Annual Thermodynamics of Materials Symposium 2018 (Sheffield, UK).

2.5.3 Johnson Matthey Case: "Predicting the Oxygen-Binding Properties of Platinum Nanoparticle Ensembles by Combining High-Precision Electron Microscopy and Density Functional Theory"

The case is based on JM research into fuel-cell cathodes. It has been published in: "Predicting the Oxygen-Binding Properties of Platinum Nanoparticle Ensembles by Combining High-Precision Electron Microscopy and Density Functional Theory", J. Aarons, L. Jones, A. Varambhia, K.E., MacArthur, D. Ozkaya, M. Sarwar, C.-K. Skylaris, P.D. Nellist; Nano Lett. 17 (2017) 4003−4012, (DOI: 10.1021/acs.nanolett.6b04799)

2.5.4 SFK Case: "Atomistic simulations of properties of lubricants"

The case study is based on the SKF's work on atomistic simulations of properties of lubricants.



2.5.5 Bosch Case: "Multi-length-scale modelling in ferroelectric Materials"

The case study is based on Bosch's contribution to the German public funded project "Multi-length-scale modelling of ferroelectric materials". It was presented at the MRS Fall Meeting 2009 (Boston, USA) and the Multiscale Materials Modeling Conference MMM 2010 (Freiburg, Germany). The report on the project is available (in German) at the following link
https://www.tib.eu/de/suchen/id/TIBKAT%3A651803438/Computergest%C3%BCtzte-Multiskalenmodellierungzur-virtuellen/.

2.5.6 DOW Case: "Modelling Drop Impact Test of Flexible Pouches Made of Thin Polyethylene Films"

The case is based on a market demand for novel and lightweight flexible food packaging replacing rigid forms of packaging, including rigid plastic, glass or metal. These "pouches" are indeed very lightweight and also do not take up much volume when disposed of. However, the value chain and end consumers have certain expectations in terms of the handling, processing, aesthetics, feel and robustness of such packaging.

2.5.7 Imperial College Case: "Machine Learning for Organic Cage Property Prediction"

The case is based on Dr Jelfs' paper "Machine Learning for Organic Cage Property Prediction", L. Turcani, R. L. Greenaway, K. E. Jelfs, Chem. Mater. 31 (2019) 714-727.
https://doi.org/10.1021/acs.chemmater.8b03572
This work was chiefly conducted by Lukas Turcani, where Dr. Rebecca Greenaway provided insight on the synthesis of cages and developed the library of precursors used for the study. The publication describes how they use machine learning to predict shape persistence and cavity size in porous organic cages.

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Contributing partners	POLITO, GCL, DPI, ANSYS-GRANTA, DOW

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Instrument	CSA
Programme	HORIZON 2020
Client	European Commission
Start date of project	01 September 2016
Duration	36 months

Consortium		
TU WIEN	Technische Universität Wien	Austria
FRAUNHOFER	Fraunhofer Gesellschaft	Germany
GCL	Goldbeck Consulting Limited	United Kingdom
POLITO	Politecnico di Torino	Italy
UU	Uppsala Universitet	Sweden
DOW	Dow Benelux B.V.	Netherlands
EPFL	Ecole Polytechnique Federale de Lausanne	Switzerland
DPI	Dutch Polymer Institute	Netherlands
SINTEF	Stiftelsen SINTEF	Norway
ACCESS e.V.	ACCESS e.V.	Germany
HZG	Helmholtz-Zentrum Geesthacht Zentrum für Material- und Küstenforschung GMBH	Germany
MDS	Materials Design S.A.R.L	France
QW	QuantumWise A/S	Denmark
GRANTA	Granta Design LTD	United Kingdom
UOY	University of York	United Kingdom
SINTEF	SINTEF AS	Norway
UNIBO	ALMA MATER STUDIORUM – UNIVERSITA DI BOLOGNA	Italy
SYNOPSYS	Synopsys Denmark ApS	Denmark

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