HEXAGON

White paper

Data science and artificial intelligence applied in the field of materials & ICME:

Accelerate innovation, accelerate generation of material data, make substantial savings!

Moncef Salmi, PhD, MBA, Solution Lead For Data Science Applied to Materials/ICME Hexagon

Executive summary

Today's highly competitive industry landscape, the economic pressure to innovate always faster, the desire to produce more customer products and the necessity to achieve significant changes to our consumer habits and production methods for ecological purposes render the industrial context ever more challenging.

In the field of engineering, pressure on research and innovation teams increases, design times shrink, businesses must rapidly adopt new and efficient Go-To-Market (GTM) strategies. In many ways, this turns in an increasing demand for more efficient modeling solutions and workflows, as well as for low cost yet highly efficient numerical material cards, and these are expected to be powered by a combination of experimental and virtual data.

In this context, Hexagon actively works on solutions that leverage Data Science (DS) and Artificial Intelligence (AI) for maximizing the power and efficiency of Integrated Computational Materials Engineering (ICME) tools and workflows.

This white paper first introduces the fundamental concepts of ICME and DS/AI to provide basic intuitions behind these two powerful technologies in the ecosystem of material innovation. Then it elaborates on some of the synergies between ICME and DS/AI, giving insights into how researchers and engineers can apply and benefit from these.

The white paper goes beyond the hype and buzz wording that one can encounter today when looking for concrete evidence about the value proposition behind DS/AI in the framework of an industrial context. It presents concrete applications of the value proposition that DS/AI tools bring in the framework of ICME and material modeling. The value proposition is summarized in three pillars: Accelerate, Assess and Optimize.

Practical examples start with how to use DS/AI for enriching material databases by maximizing the use of available material data, whether this is coming from experimental or numerical sources. An additional practical example is provided in the framework of Additive Manufacturing, addressing all three pillars of our value proposition at once. A third example focuses on Virtual Allowables and Virtual Testing of Continuous Fibers Reinforced Composites (CFRPs). Two more use cases are finally presented on the assessment of process and structural performances of parts, focusing more specifically on injection molded fiber reinforced plastics.

The practical examples section is extended to include the presentation of future applications of DS/AI in the field of Materials and ICME, conducted by Hexagon. These additional applications are focusing particularly on the field of sustainable development. A first example relates to recycling of injection molded reinforced plastics, a second example relates to the reduction of the carbon footprint of parts through a smart material recommender system, and a third example looks into light weighting in the field of eMobility via a smart material replacement system.

To complete with, it is explained how and why Hexagon the ideal strategic partner is to work with when looking to implement DS/AI powered solutions in the field of Materials and ICME, this for whichever materials, processes and scales you are interested in. The three main components of DS/AI are Simulation, Experimentation and Data - these are in the DNA of Hexagon's Materials since it was founded back in 2003!

Table of contents

1. Introduction

Today's businesses of all kinds are witnessing an unprecedented challenging environment. This complex framework imposes to all industry stakeholders to adopt fast yet efficient Go-To-Market (GTM) strategies. This implies an increasing demand for more efficient modeling chains and virtual testing tools that leverage as much as possible the available data, both experimental and numerical, for turning it into actionable insights.

The main objective of this white paper is to introduce a highly innovative yet pragmatic solution to cope with the current engineering challenges. This solution leverages the power of Data Science and Artificial Intelligence (DS/AI) technologies in the framework of Materials and Integrated Computational Material Engineering (ICME). For this purpose, an evidence-based approach is adopted in the white paper by presenting practical examples and use cases.

To start with, the basic concepts around ICME and DS/AI are presented. This aims at providing basic intuitions around these notions, i.e. DS/AI and ICME. This also aims at introducing progressively how these notions are deeply linked and highly complementary.

The white paper then provides detailed information on these concepts and solutions. Indeed, practical examples about how DS/AI is used to build a high value proposition to the market are provided. Current and future applications of Hexagon are thereafter presented, providing inspiring applications that can be built around DS/AI for Materials and ICME.

To complete with, it is explained how and why Hexagon the ideal strategic partner is to work with when looking to implement DS/AI powered solutions in the field of Materials and ICME, this for whichever materials, processes and scales you are interested in.

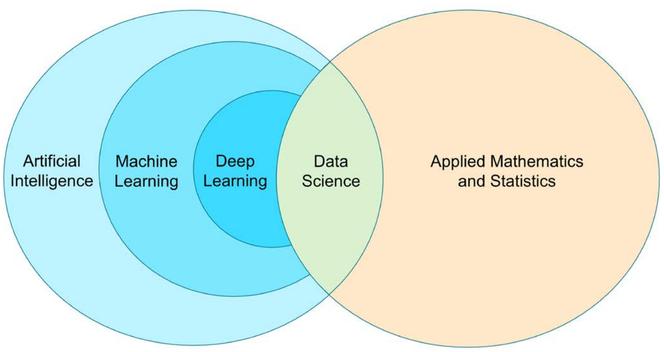

Figure 1: DS/AI general ecosystem overview

2. Main concepts

1. Data science and artificial intelligence

Although Data Science (DS) and Artificial Intelligence (AI) might appear to be very recent, first works about DS/AI started already in the mid-20th century. After two decades of active research and government funded programs on the topics, DS/AI experienced the so-called "AI Winter" in the 70s and 80s following the general disappointment of the largest worldwide funding governments, especially from the US and UK. Enthusiasm towards DS/AI grew again in the 80s thanks to a deep initiative led by the Japanese Government but Japan finally interrupted its activities in the field after about a decade of investments, again due to successive disappointments. For more information regarding AI history, one can refer to Kaplan et al (2018), Berlinski (2000), McCorduck (2004) and Russel et al (2003).

The real first success stories of DS/AI appeared in the early 2000s thanks to:

- More sophisticated models and algorithms resulting from decades of research;
- Breakthrough advancements in computational power in comparison to what was available in the 20th century;
- Unprecedented amounts of data mainly coming from the Web, IoT (Internet of things) and numerical simulation.

When speaking about Artificial Intelligence, one can hear buzzwords like: Artificial Intelligence, Machine Learning, Deep Learning, Applied Mathematics and Statistics, Data Science, Neural Networks etc. Figure 1 shows the relationship between those key terms.

AI is a global term that embeds all the fundamental and operational tools capable of mimicking the human brain behavior, e.g. learning through a trial and error process. The expectation from AI is to take decisions based on what was learned without being explicitly programmed for doing a particular action.

To illustrate this concept, let's consider a program taking an aim at recognizing an apple when parsing numerous images. Classical coding paradigms would suggest adding numerous conditions on the shape, color and texture of the objects described by the images. This can be done classically through an endless sequence of if-else statements and Boolean logics. A strong weakness of such approach is that the designer of the code may not think about all conditions which turns in a non-robust program when it comes to considering changes in the picture angle, the resolution, the average shape, etc.

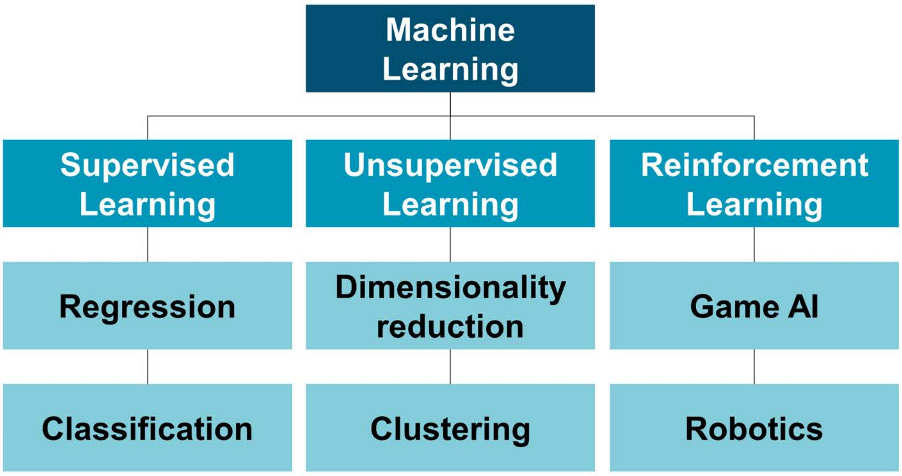

Figure 2: Overview of the main components of Machine Learning (non exhaustive representation)

This is where AI brings outstanding benefits. An AI is designed and behaves like a baby, it rapidly absorbs and assimilates data, up to a point at which it learned what an apple is about. The classical learning process of a baby is to face different situations containing apples. The baby's brain then learns how to recognize the main features representing an apple. Consequently, it becomes able to recognize an apple from a non-apple object.

An AI learns the same way. Indeed, after being showed numerous images, its neurons learn the good weights that empowers it to differentiate objects. Once the learning rate has reached a sufficient accuracy, the AI is ready for deployment and can recognize objects, even new objects that were never showed during the learning stage. Machine Learning (ML) is a subfield of AI that refers to specific algorithms and technologies. It is structured in three main families: Supervised Learning, Unsupervised Learning and Reinforcement Learning. Each of these subgroups embeds numerous algorithms as depicted in Figure 2.

- Supervised Learning: It is the ML part where algorithms perform the learning based on labeled data. An example of that is to train a ML algorithm on a database containing images of apples and pears with clear labels for each. As an outcome, the ML algorithm can recognize the right label for any similar image passed in input. It is worth noting that polynomial regression belongs to this family of Machine Learning. That means that even the simplest linear regression algorithm can be considered as a sort of Machine Learning technology.

- Unsupervised Learning: It is the ML part where the algorithm learns based on unlabeled data. Dimensionality reduction for instance is a widely used unsupervised algorithm. It consists in detecting automatically the most important statistical patterns, e.g. eigenvalues and eigenvectors among an unlabeled set of data.

- Reinforcement Learning: It can be seen as an intermediate approach between the supervised and unsupervised learning. It consists in providing the algorithm with the rules of learning through a reward function. The latter reinforces, based on the outcomes, the learning towards a given path vs. another. To illustrate this, let's take the example of an AI based chess player. It will learn the best decisions to make based on his history of wins and losses. Consequently, the more the algorithm plays, the better it becomes. Reinforcement learning is widely used in robotics and video games.

2. ICME

Part performance depends on the part's geometry, material and manufacturing process. The "holy grail" in manufacturing is to find the right technological solution for an optimal part, i.e. one with the desired set of performance targets, while reducing the design cycle, limiting the cost and increasing the output. This in an extremely challenging problem which is subjected to several severe constraints. This challenge is being addressed by multiscale-based ICME, a new paradigm which emerged just about fifteen years ago. The ICME acronym stands for "Integrated Computational Materials Engineering".

ICME, as illustrated in Figure 3, is a modeling chain which links four pillars: (i) a manufacturing process, (ii) a material's microstructure, (iii) its engineering properties and (iv) the performance of products made with it. Embedded in an optimization loop, the ICME chain can also fine-tune the process and/or the microstructures to achieve an optimal part design (e.g. reduce weight while preserving a targeted performance). For ICME to thrive in an industrial environment, it needs an efficient physical and virtual data management system.

Deep learning is a subfield of Machine Learning. It is generally based on neural networks that use many layers of neurons and this is where the term Deep is coming from. Deep Learning is widely used in Cognitive Programming like Computer Vision, Speech Recognition and Natural Language Processing. Deep Learning requires initial databases that contain tens or hundreds of thousands of data points. This represents orders of magnitudes more of required input data than Shallow Learning or classical Machine Learning. On the other hand, Deep Learning is highly powerful when dealing with complex and/or big amounts of data.

DS/AI rely heavily on applied mathematics, statistics and computer science. DS/AI can be seen as a more trendy and catchy term for applied mathematics and statistics. Indeed, the basic tools behind DS/AI exist already since few decades, if not centuries.

Finally, Data Science can be seen as the intersection between all the latter fields. Data Science is the most global term that embeds at the same time: AI, ML, Deep Learning, applied mathematics, statistics and computer science. This is in a nutshell a very general overview of the main concepts related to the DS/AI ecosystem. It is important to have a sane intuition about DS/AI to understand objectively and efficiently its value proposition in the framework of materials, ICME, modeling and numerical simulation.

For more information and details regarding the main notions and components of DS/AI, it is recommended to document yourself with the following sources: Bishop (2006), Brazdil et al (2009), Samuel (1959) and Kohavi et al (1998).

ICME is powerful as it augments the design optimization space, it significantly increases modeling accuracy, and it results in significant design savings. It allows mastering fully the material-manufacturing-part performance chain, computing and optimizing part performance as a function of upfront materials and processing factors. It also accelerates the Go-To-Market (GTM) process as it maximizes chances of fulfilling product specifications (e.g. prevent extra expensive design loops), which is not well guaranteed by a classic design & engineering process due to erroneous assumptions and simplifications.

The ICME ecosystem chains four major components. Let's illustrate this through two examples: Injection Molded Fiber Reinforced Plastic Parts, and Additively Manufactured Parts. The examples are summarized in Table 1.

Consequently, a strong value proposition of ICME is to connect the dots among the numerous material and processing stages of a product, at different levels and scales.

ICME deals with large amounts of data of various types, being experimental or numerical. Consequently, DS/AI is an obvious candidate for empowering ICME and pushing its limits even further. The next section of this white paper will step into how ICME can interact with DS/AI for synergetic effects.

For a deeper dive into ICME, the reader is kindly referred to Doghri et al (2020). For more details about ICME, the reader is kindly referred to the following sources: Allison (2006, 2011), Chopra (2015) and Cowles et al (2010).

3. DS/AI for ICME

The four pillars of ICME involves using two types of data: Experimental and Virtual data. On the one hand, experimental data has a great degree of credibility in the minds of stakeholders. It relates to the real world and brings evidences which are hard to deny by any stakeholder belonging to the product lifecycle. Experimental data

Stages	Use Case #1: Injection Molded Fiber Reinforced Plastic Parts	Use Case #2: Additively Manufactured Parts
Manufacturing Process and its Influencing Factors	Injection Molding. Mold/melt temperatures and pressures, injection gate position, flow rate, the material properties.	Additive Manufacturing. Print direction, toolpath, printing speed, thermal conditions during print, layer thickness, etc.
Material Microstructure	Fiber orientation state, presence of local weldline, fiber length and fiber content distribution over the part, porosity, etc.	Lattice structure, bead size characteristics, voids and local defects, toolpath, multilayered microstructure, local defects, etc.
Material Engineering Properties	Anisotropic properties such as stiffness and strength, dependent on local fiber orientation, weldline, etc.	Anisotropic properties such as stiffness and strength, dependent on the local lattice geometry, partial infill, toolpath, orientation of the fibers, etc.
Final Product Performance	Warpage, stiffness, load at break and location of failure dependent on how the part is precisely injection molded.	Warpage, stiffness, load at break and location of failure dependent on how the part is precisely 3D printed.

Table 1 : Examples of ICME Applications

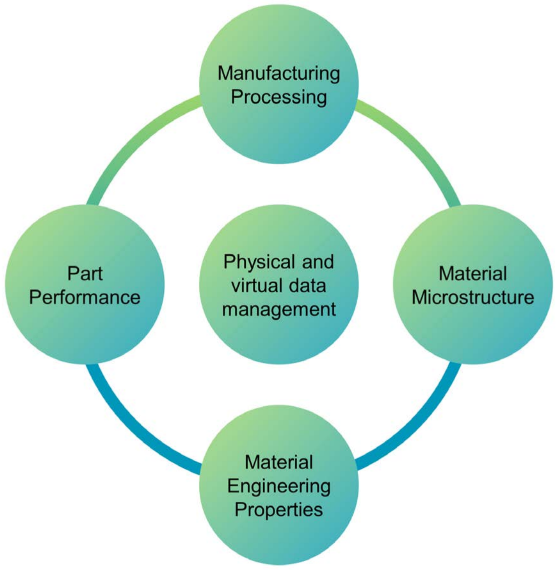

Figure 3: ICME concept

is however expensive to produce both budget and time wise. Consequently, relying solely on experimental data to characterize a material, design a part, test out prototypes, tune manufacturing settings etc. is not a valid track. On the other hand, simulation data is generally cheaper to produce both from time and budgeting standpoints. That said, it requests particular expertise, highly qualified workforce a dedicated IT infrastructure with computational power. And very often, virtual testing must be fed with real experimental data to develop high fidelity models and results.

This is exactly where DS/AI can bring a great value to ICME:

- Better designing initial Design of Experiments (DoE) related to experimental data.
- Detect automatically statistical patterns between the different sorts of data at the different stages of the ICME process.
- Make the computational cost of virtual testing more efficient by using the adequate DS/AI tools like dimensionality reduction, reduced modeling, etc.
- Embed expertise into learned DS/AI algorithms.
- Automate complex workflows in an efficient way.

Consequently, when merged altogether, DS/AI and ICME becomes a highly powerful and complementary solution.

3. Industrial context

1. Challenges

Today's highly competitive industry landscape, the economic pressure to innovate always faster, the desire to produce more customer products and the necessity to achieve significant changes to our consumer habits and production methods for ecological purposes render the industrial context ever more challenging.

In the field of engineering, pressure on research and innovation teams increases, design times shrink, businesses must rapidly adopt new and efficient Go-To-Market (GTM) strategies. In many ways, this turns in an increasing demand for more efficient modeling solutions and workflows, as well as for low cost yet highly efficient numerical material cards. These are expected to be powered by a combination of experimental and virtual data.

2. Value proposition

Given the current global business ecosystem and challenges presented in the previous section, and based on the above definition of ICME and its empowerment using DS/AI, the DS/AI empowered solutions seem to be a great candidate and a well-suited immediate solution to many engineering challenges. In short, their main value proposition can be summarized as depicted in Figure 4: Accelerate, Assess and Optimize.

Indeed, DS/AI empowered ICME has the ability to leverage the best of the 2 worlds: Experimental testing data and Virtual Testing Data. This is a solution for reducing the Go to Market (GTM) lifecycle. This is achieved by better selecting the best suited experimental campaigns to be used for assessing the material and product performance at different stages.

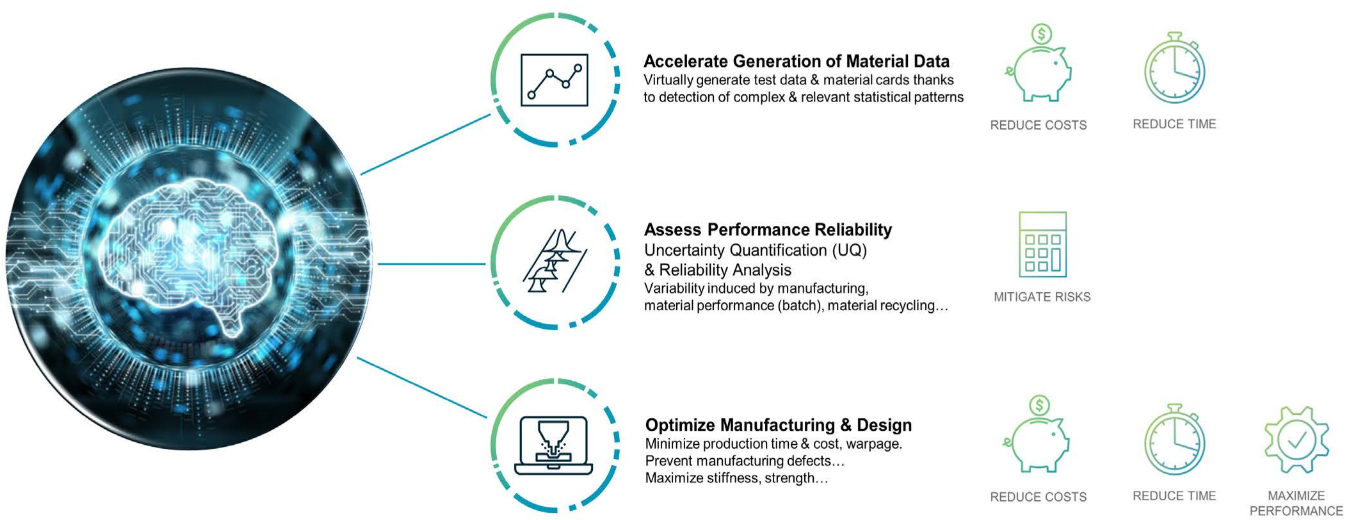

Figure 4: DS/AI for ICME value proposition

DS/AI empowered ICME leverages the best of the two worlds: Experimental Testing Data and Virtual Testing Data. The ability of DS/AI to detect efficiently complex statistical patterns makes it possible to extract as much insights as possible from all types of data. This can be used to optimize the definition of experimental test matrices and, most importantly, to virtually generate new material data at a fraction of the classical characterization efforts. This way one can expand the coverage of a material database, produce data for material systems that have been barely characterized (e.g. various fiber contents, temperatures, strain rates, recycled rates etc.), sometimes still under development.

The ability of DS/AI to run efficiently virtual testing and linking different levels and scales also provides the possibility to establish direct links between the process parameter and the final product performance. Consequently, the latter workflow enables determining the best processing parameters for optimizing part performance, no matter what that depends upon.

All in all, well-developed and trained DS/AI engines delivers accurate results at a fraction of the classical budget and time resources, this in a large variety of fields and applications. This automatically turns into significant GTM time savings.

After looking at the main concepts and intuitions around DS/AI empowered ICME, it is now time to leave fundamentals and theories aside and step into practical examples around the concrete activities Hexagon is carrying out for the future delivery of new commercial DS/AI empowered ICME solutions.

4. Practical applications

1. Material database enrichment

Material data is a necessity in the field of engineering, it is at the heart of all activities: material research and innovation, manufacturing, design and engineering. And as soon as you step into computer aided engineering (CAE), material cards are required which means material data must be produced to calibrate the cards.

Material data represents a key asset for most companies including OEMs, Tier 1, Tier 2 and material suppliers. Generating experimental material data is expensive from financial, human or time perspectives. In this framework, virtual testing is a great candidate for building exhaustive material databases (DBs).

Virtual material testing can be complex and computationally heavy. Accuracy can also be a challenge, depending on the material system and the properties to compute. Finally, material calibration with respect to reference experimental data is a repetitive process that can be overwhelming.

DS/AI brings a solution that overcomes the above-mentioned pain points related to virtual testing, while keeping all its benefits. DS/AI allows accelerating the generation of material data at minimal cost.

When applying DS/AI for enriching material DBs, several workflows and solutions can be considered. These are at a high level summarized in Figure 5.

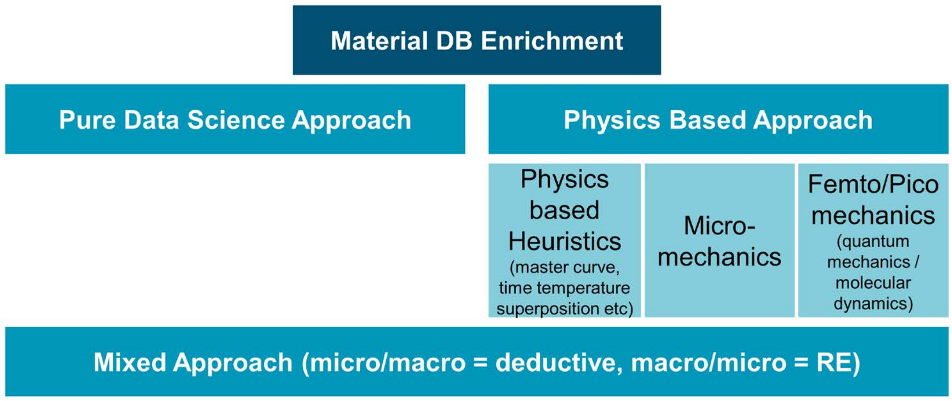

Figure 5: Different workflows for Material Database Enrichment

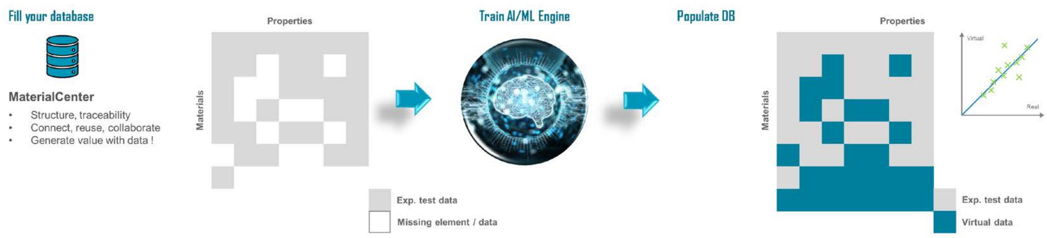

Figure 6: Material Database Enrichment using a pure data science approach

Three main paths can be adopted in this perspective:

- A pure data science approach where the correlations and statistical relationships and patterns are detected automatically between the different materials and their properties
- The Physics based approach: This takes into account some physics based laws like:
    - o Master curves expressing the evolution of a given property as function of external conditions
    - o Multiscale approaches like homogenization whether mean field based or full field based
    - o Quantum mechanics and molecular dynamics at lower scales
- The mixed approach leveraging the power of the two above

In this first example, a pure Data Science approach is adopted. An initial "holed matrix" containing the initial material database is considered. A holed matrix contains typically in one axis the different material grades considered and in its other axis the corresponding properties. Generally, one ends up with a holed matrix since all properties are not computed for all materials. The aim of this first example is to detect the correlations and relationships automatically in order to fill the gaps.

This is done by using different DS/ML tools like regression, correlation detection, reduced order modeling until filling the gaps progressively. The final result is a fully filled matrix with all properties for all materials. This general concept is represented by Figure 6. A more detailed workflow, with the corresponding results at each step, is reported by Figure 7.

For those who start material testing from scratch on a given family of materials, DS/AI can be leveraged to create a smart test campaign which combines experimental and virtual testing.

Large test campaigns with strong relationships between the measurements are highly suitable to this smart characterization approach that provides significant characterization savings.

The specific exercise illustrated on Figure 8, performed on a new family of recycled materials being developed for greater sustainability, does provide 40 % savings. Given that such test campaigns cost around 250-500 k€ depending on several testing factors, the return on investment (ROI) of AI/ML is significant! (>100 k€).

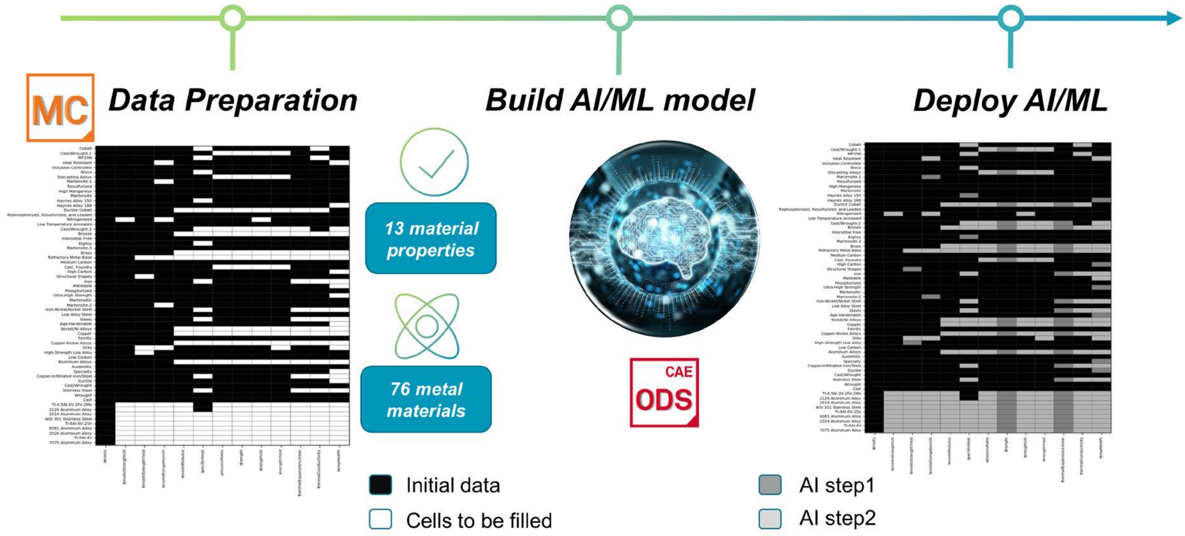

Figure 7: Workflow for Material Database Enrichment using a pure data science approach

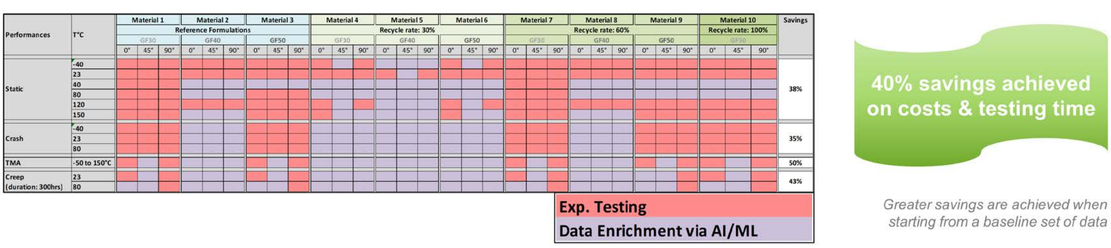

Figure 8: Example of a smart test campaign produced on a family of 10 fiber reinforced thermoplastics (mix of neat and recycled formulations for different recycled rates and fiber contents; various performances and testing temperatures)

The second example aims at adding physics in the workflow. Indeed, physics-based considerations such as master curves and homogenization-based material modeling tools can be added to expand the power and accuracy of the DS/AI tools. This enriched workflow can for instance be used to perform smart physics-based interpolations of material properties (e.g. time-temperature dependencies of plastics), either at macroscopic or at lower scales.

Once this is done, material modeling and homogenization methods can be used to virtually populate and expand, exhaustively, the input material database with data at varying tests conditions, that were not even necessarily addressed in the input material database.

Another use case with the mixed approach here described is to perform smart calibration of material cards (both macroscopic and constitutive phase properties), accelerating the delivery of CAE material cards.

This general concept of a mixed approach is represented in Figure 9. A more detailed workflow, with illustrative results at each step, is reported in Figure 10.

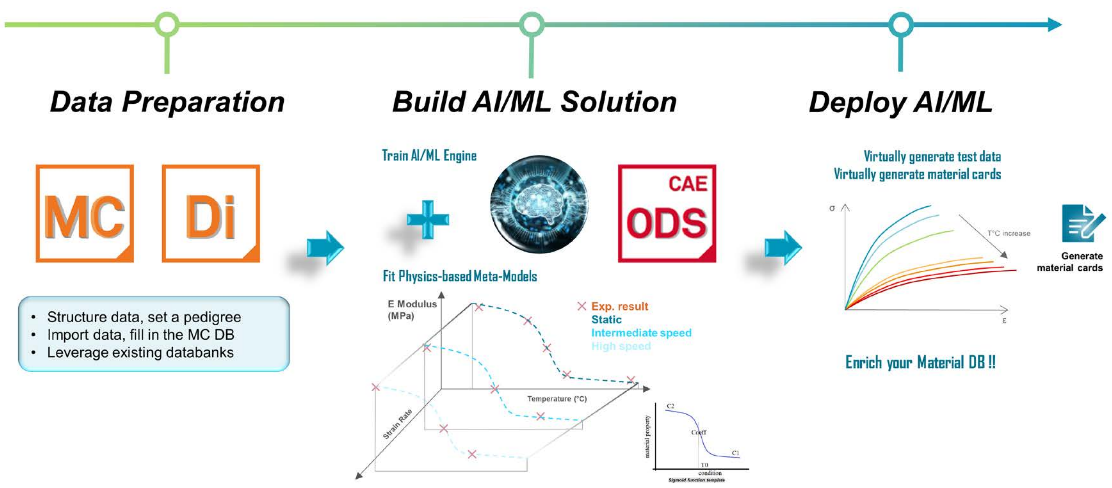

Figure 9: Material Database Enrichment using a mixed approach

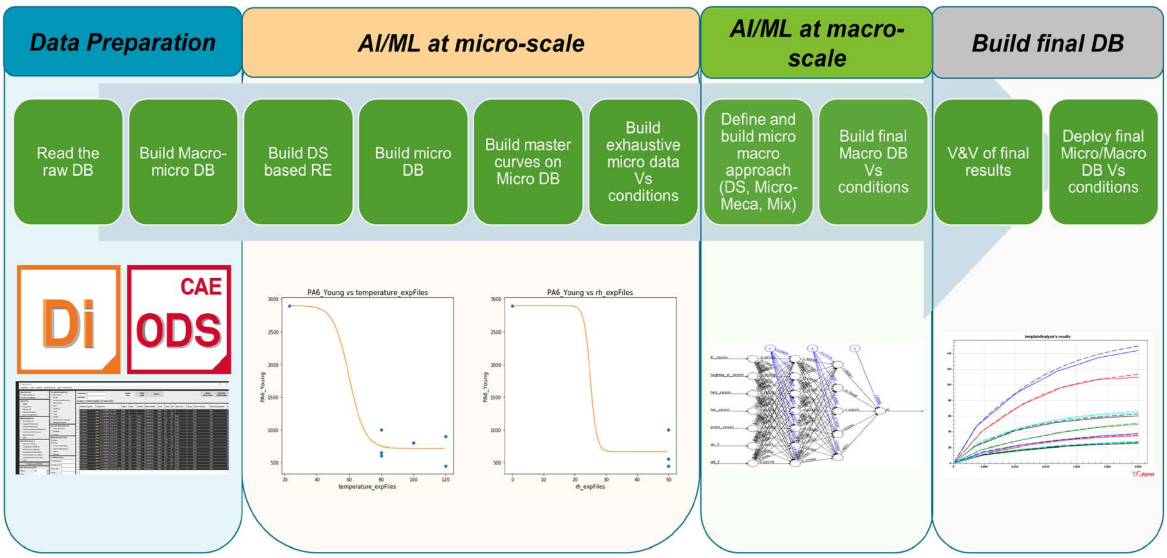

Figure 10: Workflow for Material Database Enrichment using a mixed approach

2. Additive Manufacturing

Additive Manufacturing (AM) is a breakthrough technology for many businesses and organizations. However, a lot of unknowns as well as variability in material and part performances are still experienced daily in this field. For high end additive parts, virtual testing is of great interest to better control and optimize the AM process quality, minimize print time, and maximize the end performance of parts. For this purpose, finite element modeling is increasingly being considered, even though it can be numerically complex to model and expensive to compute, depending on the part and properties at stake.

DS/AI brings at this level a solution that overcomes the above-mentioned pain points related to virtual testing for AM, by keeping all its benefits at the same time.

In the provided example, a DS/AI workflow is implemented for predicting the warpage of a 3D printed part based on the AM processing parameters. The AM process considered for this exercise is SLS; other processes could of course be considered too. The following process parameters were considered for this application: laser power, scan spacing and scan speed.

A typical AM simulation takes between from a few minutes to a few hours, depending on the part complexity. The proposed DS/AI workflow suggests running a reduced amount of high-fidelity AM simulations, typically 20 simulations. Once the high-fidelity database is ready, a reduced order model is computed. The reduced order model allows predicting warpage or deflection at various locations on the printed part for any combination of printing parameters. As shown in Figure 11, the reduced order model predicts with high accuracy the local deflections on the considered test data. Such a DS/AI model can then be used for optimizing the AM process parameters regarding warpage at almost no computational cost, thanks to the DS/AI layer.

3. Virtual Allowables of CFRPs

Continuous Fiber Reinforced Composites (CFRPs) are heavily used in aerospace and defense industries for their high stiffness and strength to density ratios. These industries are extremely demanding in terms of controlling the variability of the composite properties as a function of the manufacturing process, material batch, layup definition and various loading conditions, sources of variability and potential presence of defects. Characterizing experimentally all of these is highly expensive time wise and financial wise.

For this reason, virtual testing of CFRPs for the purpose of computing Virtual Allowables provides substantial value. However, virtual testing of CFRPs is rather complex as the physics involved are themselves complex. It also requires expertise to master the various sources of variability that must be characterized for the input definition of the virtual VA analysis workflow. Lastly, solving large test campaigns can be computationally expensive.

In this application, Digimat-VA – Hexagon's high-fidelity virtual testing tool for CFRPs – is used to perform high fidelity failure predictions of various CFRPs coupons configurations (loads, layups, environmental conditions, etc.).

Digimat-VA offers two main solutions for assessing the failure of virtual CFRP coupons. A first model, called here failureModel1, that assesses the failure limits of coupons at a classical computational cost, i.e. of the order of minutes to hours. A second model, called here failureModel2, being more accurate than the first one but computationally more expensive (VA campaign costs dozens of hours).

Then, DS/AI tools are used to build a surrogate model that complements Digimat-VA to virtually generate a larger amount of material data on configurations that were not numerically computed. In this application, Hexagon created

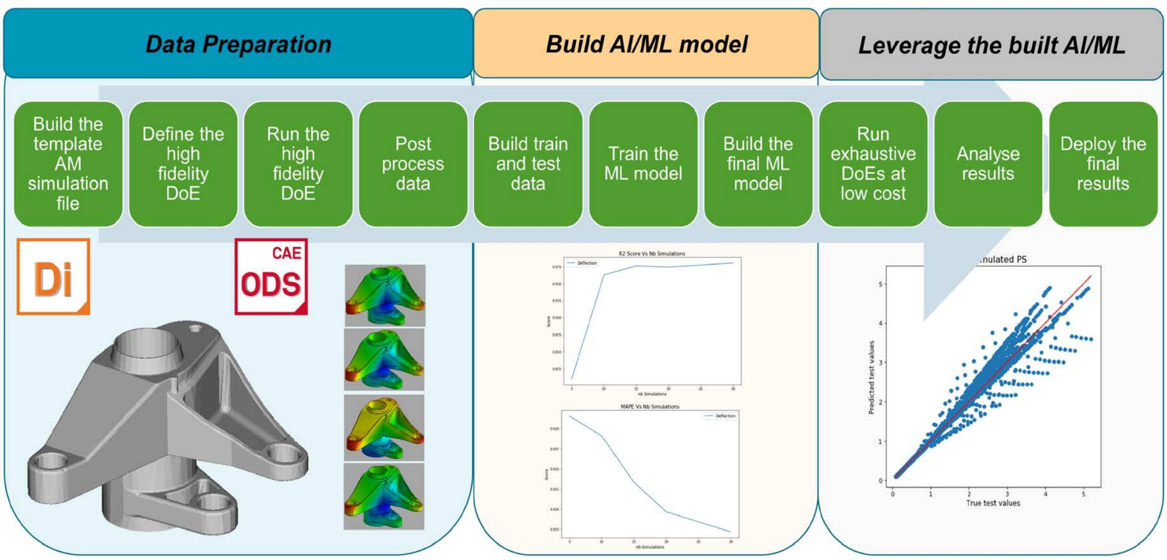

Figure 11: Workflow for DS/AI applied to Additive Manufacturing

a Deep Learning model that reproduces the outcomes of the high fidelity failureModel2, at a fraction of its computational cost. In this purpose, a high-fidelity database with 15000 Digimat-VA simulations using failureModel1 and 120 Digimat-VA simulation using failureModel2 is built. The computational cost for building such a database is equivalent to 50 days of computation time. The idea behind the implemented solution is to build a first neural network that mimics the functioning of failurreModel1 using the 15000 data points. The second step is to build a “corrective” second neural network that reduces the gap between failureModel1 and failureModel2 predictions based on the 120 data points using failureModel2. The general iterative algorithm combining the two neural networks is depicted in Figure 12.

After several iterations between the two neural networks, the final DS/AI model mimics accurately the behavior of failureModel2. The final model is then able to not only rebuild the 15000 initial data points but goes beyond: using the failureModel2 based neural network, thousands of extra data are computed in a few seconds compared to days of computation work. A detailed representation of the workflow, with the corresponding results at each step, is reported in Figure 13.

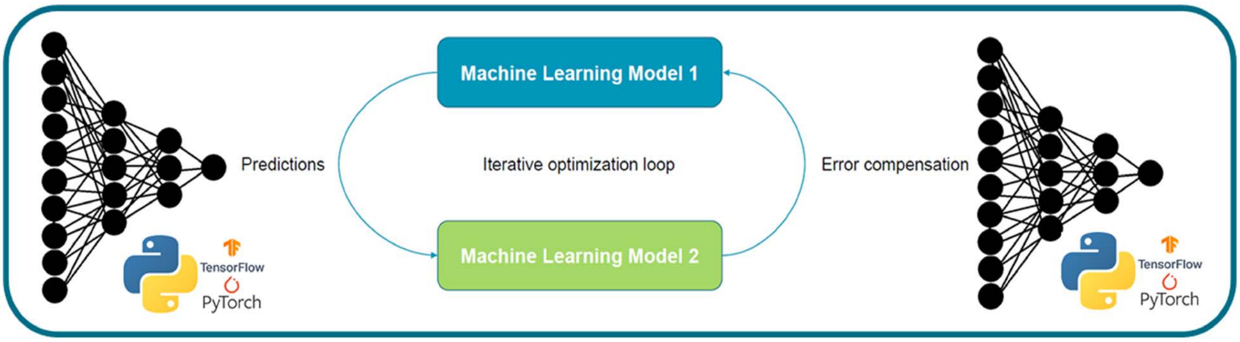

Figure 12: Iterative neural network approach applied to Virtual Allowables

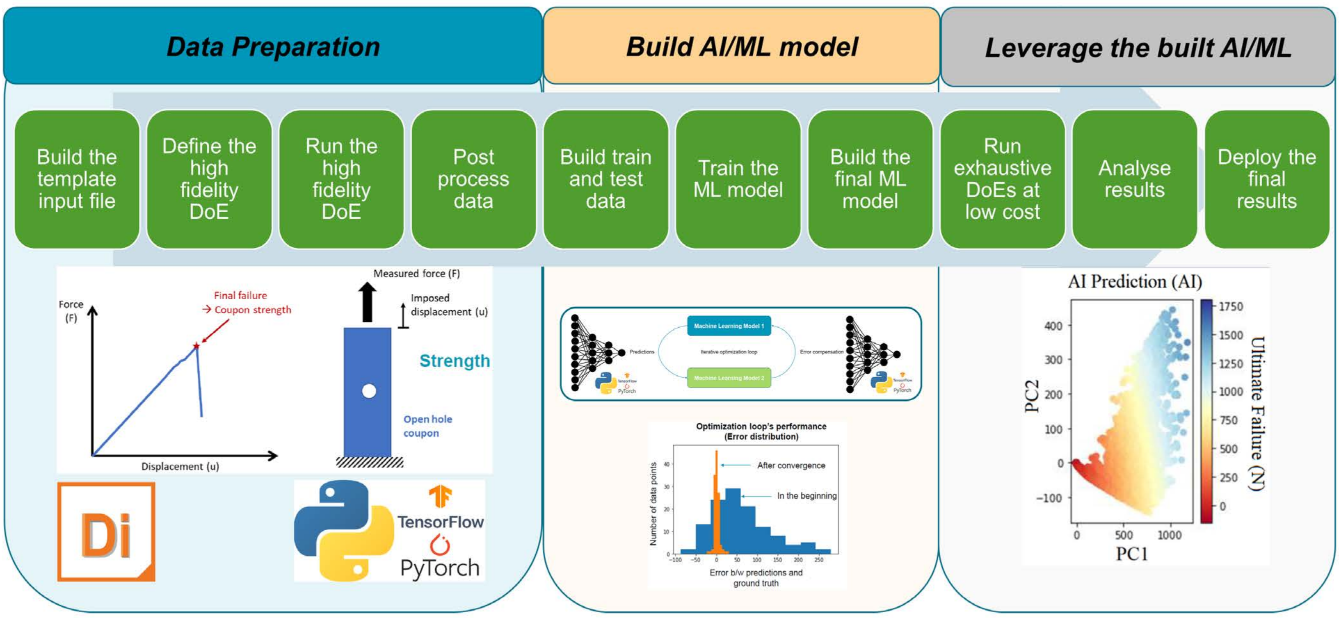

Figure 13: Workflow for DS/AI applied to Virtual Allowables

4. Process to structure: Reliability analysis

One of the base principles and value propositions of ICME is to link the end part performance to the manufacturing process. The current application focuses specifically on the case of injection molded fiber reinforced plastics, as illustrated in Figure 14.

When numerically designing a structural part, the typical high level numerical ICME workflow is broken down in five main steps, as depicted in Figure 15:

1. Design the part, prepare the CAD. Topology optimization may be performed.
2. Mesh the part, prepare the structural finite element model for load cases of interest.
3. Simulate injection molding for a given set of processing parameters: gating positions, thermal conditions, injection time, material properties, etc.
4. Perform structurally coupled Digimat to FEA analyses.
5. Analyze the failure index output at each location of the part, for each given load case and conclude on the overall performance of the studied part.

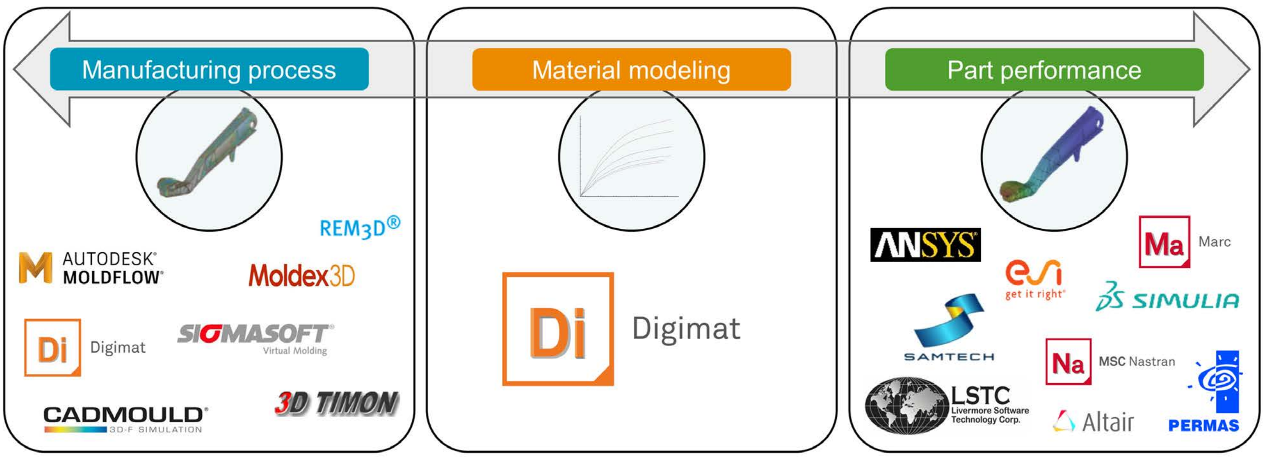

Figure 14: ICME in the field of injection molded fiber reinforced plastic parts

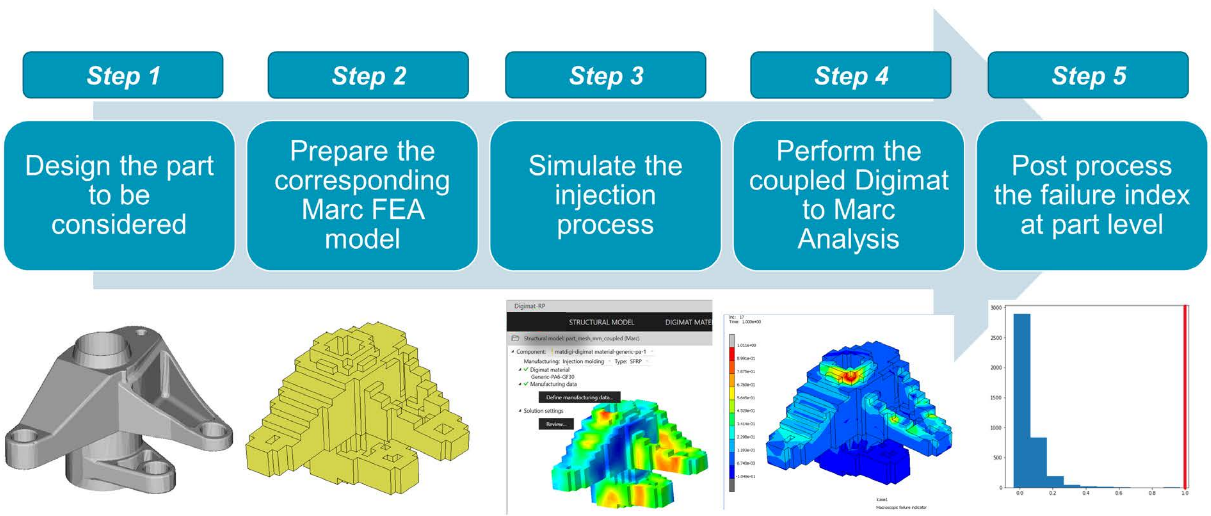

Figure 15: High fidelity ICME computation chain from injection process simulation to part performance assessment

With this application, DS/AI is used to establish a direct link between the injection molding parameters and the final local failure index output, at each location of the part for a given load case. As reported in Figure 16, the diagonal curve shows the high agreement between the predicted failure indices at part level for some given injection process parameters with respect to the reference test data that the model never saw during its learning stage.

Once the model is ready, it is used for assessing the probability of part's failure, hence its reliability, for a given uncertainty on the local orientation tensor prediction that would result from variability (expected or unexpected) on the processing input. The final curve in Figure 16 reports the evolution of the probability of failure as function of the orientation tensor uncertainty.

This shows how important it can be to take manufacturing uncertainties into consideration for designing parts in a more robust fashion. Indeed, it reduces risk that a part does not ultimately meet technical specifications because final production deviates from how it was originally intended to be produced.

5. Process to structure: Sensitivity analysis

This application is an extension of the previous one, the main goal being here to assess the sensitivities of the final part performance, e.g. local failure index, to input processing parameters such as the gating positions, thermal conditions, flow rate, material properties, etc. Ultimately this can turn into the optimization of processing for maximizing the end performance of the part.

This kind of investigation is used to assess quantitatively what are the most important processing parameters for a given targeted performance. A typical example of how that can be used by engineers and designers is to leverage this kind of DS/AI based investigation in conjunction with a Pareto Analysis for identifying what is the best machine configuration based on an outcome/cost ratio. It also allows the identification of the most critical process parameters so that the manufacturing/production team can work on it and optimize manufacturing. Sensitivity analyses are also a key step in quality assurance protocols and frameworks like the Six Sigma Methodology. A detailed representation of the workflow, with the corresponding results at each step, is reported in Figure 17.

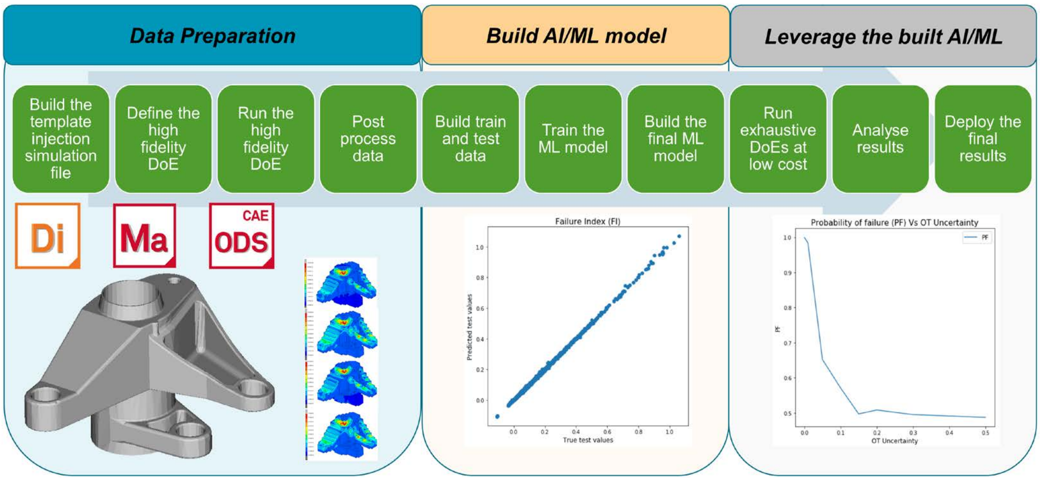

Figure 16: DS/AI workflow for carrying out Reliability Analyses on the performance of injection molded fiber reinforced plastic parts

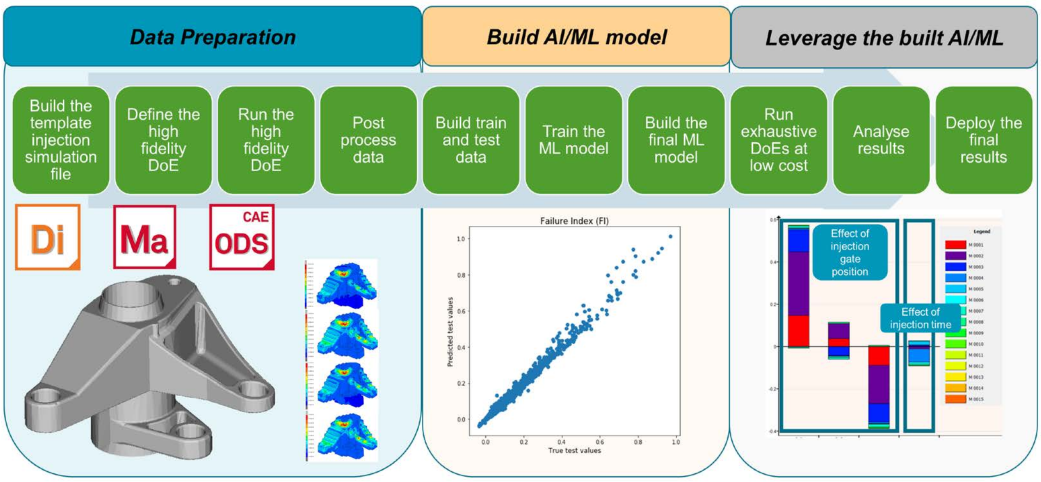

Figure 17: Workflow for DS/AI applied to Sensitivity Analysis for injection simulation

5. Future application tracks

1. Recycling

In the field of injection molded plastic parts, cold runners and sprues can be recycled while manufacturing parts. The rising importance of sustainability in engineering & manufacturing leads to considering this option even for semi-structural and structural applications. The recycling process tends to break fibers and depending on the techniques along with the recycled rates being considered, the material performance can significantly vary to a point it no longer meets technical specifications.

Interesting questions suddenly arise: How can we efficiently determine the optimal trade-off between recyclability and part performance ? What is the maximum recycling rate one can allow without altering the part performance by more than X % ?

This is a very interesting avenue for DS/AI where Hexagon can step in. The proposed approach is to implement a standalone cross-disciplinary ICME solution, powered by Digimat and DS/AI technologies, that

1. Assesses the reliability of a manufactured part, in terms of stiffness, load at break etc. as function of the recycling rate being considered;
2. Determines the optimal recycled rate for a targeted minimum part performance.

A similar workflow to the one presented in the Practical Examples section would be adopted to roll this out.

2. Reducing carbon footprint

Carbon footprint during the product lifecycle is a major concern in today's industries. The overall lifecycle of the consumed materials impacts the final carbon footprint of any given product.

The use of DS/AI could serve a design engineer to down select the most suitable material for a given application and set of requirements by considering the material carbon footprint into the design optimization loops. Such application would also address the concern of how a design engineer can, for an application currently under production, identify material alternatives to the currently utilized one that reduce the overall carbon footprint of the fabricated product.

A DS/AI solution Hexagon can here look into is a smart material recommender system designed with the purpose of reducing the carbon footprint of any given product. The carbon footprint optimization would be structured around three strategic pillars:

- The richness of a structured material lifecycle assessment database >> MaterialCenter
- DS/AI efficiency in detecting complex patterns through dimensionality reduction
- ICME powered by the Digimat multiscale modeling technology

3. Light weighting for eMobility

For ecological reasons, the eMobility industry has in a few years become a massive paradigm shift in one of the biggest industries ever, the automotive industry not to generalize to the transportation industry as a whole. Electric engines are gaining momentum and will in a few years only dominate the historical fossil fuel engines. To augment their autonomy, significant weight optimization is required to balance out the additional weight of electric batteries.

On this specific topic, Hexagon can implement a DS/AI solution that precisely addresses this design optimization topic by playing not only on the design of parts but also on the material selection using a smart material recommender system, reduced modeling and deep learning.

6. Hexagon: Your strategic partner for DS/AI applied in the field of Materials and ICME

The application of DS/AI for Materials and ICME relies on three main building blocks: Experimenting, Simulating and Data Leveraging. As illustrated in Figure 18, Hexagon is focused on delivering autonomous solutions to its customers by connecting the physical and the virtual worlds together. As such, Hexagon is structured and focused towards addressing these three building blocks.

- Experimental: Testing is a key ingredient of DS/AI and drives solution accuracy. Hexagon has deep experience in the field thanks to its whole metrology division, its Volume Graphics technology to post-process CT scans, and its experience & expertise in performing complex experimental test campaigns for characterizing materials and parts. Do not hesitate to reach out to us for assisting you on this! And when it comes to characterizing materials, you can count on us to help you optimally define your test campaigns, designing them smartly so they fit best in a AI/ML framework.
- Simulation: Hexagon's Manufacturing Intelligence division is all around simulation for the purpose of virtually mimicking physical behaviors. In the field of Materials and ICME, Hexagon is an industry pioneer in developing advanced material modeling, micromechanics and integrative modeling solutions, this being at the heart of Digimat since its foundation. Digimat software

DS/AI side, Hexagon is dedicated to the development of DS/AI solutions and working hand-in-hand with Materials and ICME to implement cutting-edge solutions. Finally, to empower teams to develop the most powerful DS/AI solutions, Hexagon acquired and now commercializes Odyssee - a strong AI/ML technology.

- **Data enabling:** Data is often the most valuable asset of a company, no matter what field it is in. Data is at the core of any DS/AI solution, it is strategic to manage the data, structure it, have full traceability on it, share it between stakeholders etc. For this purpose, Hexagon develops among others MaterialCenter, a material data management platform best positioned to assist you in that journey.

For all of these reasons, be assured that Hexagon is THE strategic partner of choice for developing DS/AI solutions you are looking for, especially in the field of Materials and ICME as was shown in this white paper.

To end with, let's remind that the three major building blocks of DS/AI to materials and ICME all show in the 10X ICME initiative, as illustrated in Figure 19.

For a deeper dive into the 10 components of the 10X ICME initiative, the reader is kindly referred to Doghri et al (2020). illustrated in Figure 19.

For a deeper dive into the 10 components of the 10X ICME initiative, the reader is kindly referred to Doghri et al (2020).

Figure 18: Hexagon strategic focus on the road to autonomous solutions

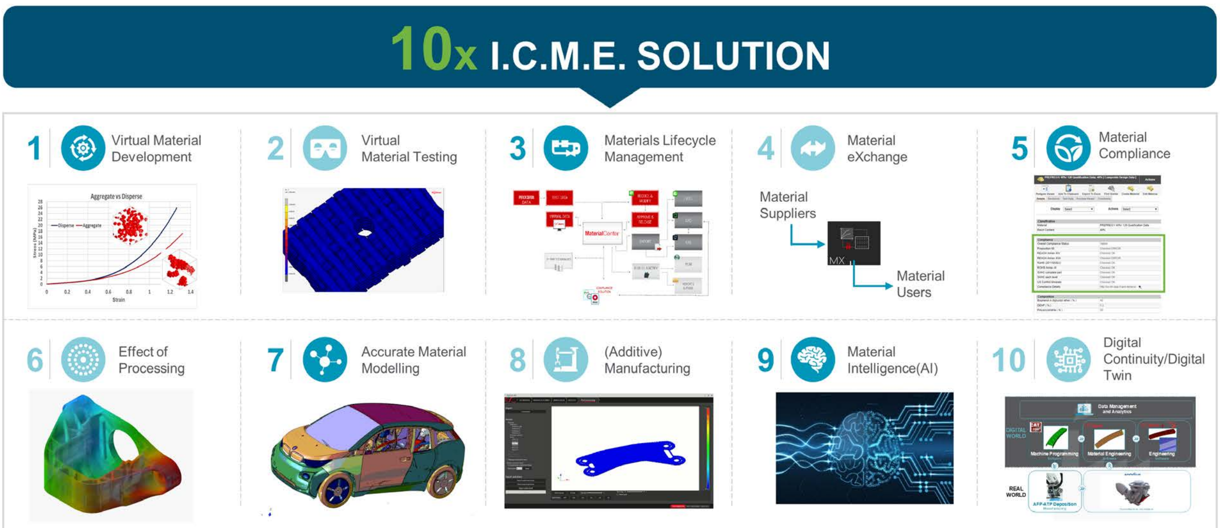

Figure 19: 10X ICME initiative

Conclusions

DS/AI is a powerful technology and a key enabler to accelerate innovation in the field of materials and ICME, as well as to accelerate the generation of material data. The main value propositions in the realm of materials and ICME are: Accelerate, Assess and Optimize.

As it has been viewed, DS/AI is a strategic tool for performing more efficient numerical and experimental DoEs. This allows to shorten the overall GTM time of new products. DS/AI also allows to leverage more efficiently and accurately the mix of experimental and numerical data companies continuously generate. All this is done through technologies such as dimensionality reduction, neuronal networks, autoencoders and reduced modeling to name a few. Finally, optimization is an obvious application of the efficient and accurate DS/AI based models once built using the gathered experimental and/or numerical data.

Based on the presented concepts, practical examples Hexagon applied so far as well as some insights into the future vision of Hexagon were presented, proving that Hexagon has experience in this field and actively assists customers in developing solutions along those lines.

If interested in any of the topics presented in this paper, reach out to Hexagon to learn more and initiate discussion around how Hexagon can help you address your needs and challenges!

References

1. **Allison, J.** (2011): Integrated Computational Materials Engineering (ICME): The Next Big Thing in Materials. Seminar, "Materials Information luncheon", August 3rd, www.youtube.com (ChannelTMS).

2. **Allison, J.; Backman D.; Christodoulou L.** (2006): Integrated Computational Materials Engineering: A New Paradigm for the Global Materials Profession. JOM (TMS).

3. **Alpaydin, E.** (2020). Introduction to Machine Learning (Fourth ed.). MIT.

4. **Arthur, S.** (1959): Some Studies in Machine Learning Using the Game of Checkers. IBM Journal of Research and Development.

5. **Berlinski, D.** (2000), The Advent of the Algorithm, Harcourt Books.

6. **Bishop, C. M.** (2006), Pattern Recognition and Machine Learning, Springer, ISBN 978-0-387-31073-2.

7. **Brazdil, P.; Carrier, C.G.; Soares, C.; Vilalta, R.** (2009): Metalearning: Applications to Data Mining. Springer Science & Business Media.

8. **Chopra, N.** (2015): Integrated Computational Materials Engineering: A Multi-Scale Approach.

9. **Cowles, B.A.; Backman D.** (2010): Advancement and implementation of integrated computational materials engineering (ICME) for aerospace applications. Preprint AFRL-RX-WP-TP-2010-4151.

10. **Doghri, I.; Adam, L.** (2020) : Integrated Computational Material Engineering (ICME) for beginners.

11. **Kaplan, A.; Haenlein, M.** (2019). "Siri, Siri, in my hand: Who's the fairest in the land? On the interpretations, illustrations, and implications of artificial intelligence". Business Horizons.

12. **Kohavi, R; Provost, F.** (1998): Glossary of terms, Machine Learning.

13. **McCorduck, P.** (2004), Machines Who Think.

14. **Russell, S. J.; Norvig, P.** (2003), Artificial Intelligence: A Modern Approach, Upper Saddle River, New Jersey.

Hexagon is a global leader in sensor, software and autonomous solutions. We are putting data to work to boost efficiency, productivity, and quality across industrial, manufacturing, infrastructure, safety, and mobility applications.

Our technologies are shaping urban and production ecosystems to become increasingly connected and autonomous – ensuring a scalable, sustainable future.

MSC Software, part of Hexagon's Manufacturing Intelligence division, is one of the ten original software companies and a global leader in helping product manufacturers to advance their engineering methods with simulation software and services. Learn more at mscsoftware.com. Hexagon's Manufacturing Intelligence division provides solutions that utilise data from design and engineering, production and metrology to make manufacturing smarter.

Learn more about Hexagon (Nasdaq Stockholm: HEXA B) at hexagon.com and follow us @HexagonAB.