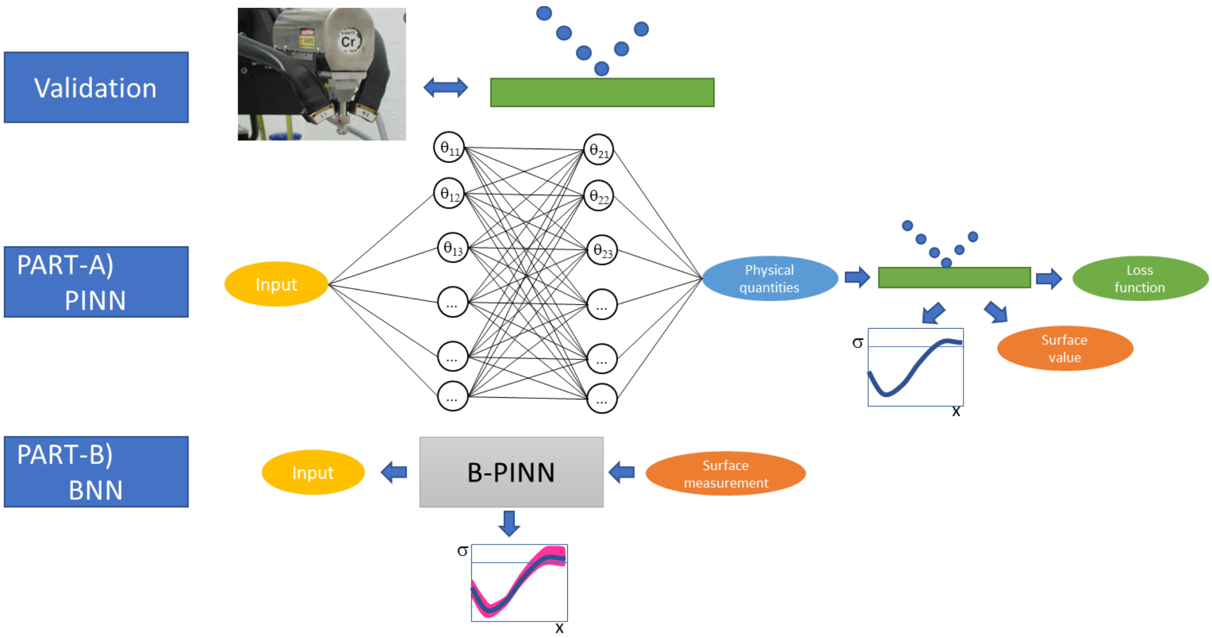
REAL TIME INDUSTRIAL APPLICATION OF NEW AI HYBRID MODELS



MOTIVATION

Research and innovation in materials science is a fundamental key for a sustainable technological and industrial development in Europe. New materials and new manufacturing processes lead to new industries, new technologies, new business models and, also, new challenges. Nowadays, materials science must deal with complex materials and advance manufacturing process which require new methodologies for material modelling and characterization.

Artificial intelligence has been changing most areas of industrial technology during the last and present decades, as a part of the so-called Industry 4.0 revolution. The automation, the introduction of smart and autonomous systems and the implementation of complex controllers have strongly influenced manufacturing and process facilities. One area where artificial intelligence, and in particular deep learning, offer a big potential is quality control. The application of smart cameras on production lines has automated quality inspection, which was otherwise done manually. This has increased the production speed and product reliability, while simultaneously reducing manufacturing time and cost. Manufacturers have been using cameras in **quality control** applications for many years, but the joining with deep learning represents a jump from earlier technologies. The combination of measurements, multiphysics/multiscale modelling and ML or DL will further amplify the information obtained, framing the problem, and giving a powerful tool for decision making.

Data driven models are considered a new paradigm in Material Science [1][2]. The power of big data, machine learning, artificial intelligence, data management, open data… is not completely applied in data-driven materials science. New branches such as materials informatics or **hybrid modelling** are emerging thanks to supercomputers and high-performance algorithms that make it possible to manipulate huge amounts of data. The **hybrid models** are powerful alternatives to physical modelling leveraging the innovations in Machine Learning (ML) and Deep Learning (DL) offering a **real time** solution for quality control.

ADVANCED MATERIAL SIMULATION company aspires to develop and validate a new and original hybrid modelling methodology based on the combination of advanced modelling, and artificial intelligence The methodology will be applied to industrial manufacturing levels to maximize the information extracted from testing, developing new real time tools.

METHODOLOGY

Some NN architectures have been identified as potentially useful in hybrid modelling combining data-driven with physical laws; for example, surrogate models, Bayesian neural networks, and Physics informed neural networks. The tight link between machine learning and multiscale modeling is a two-way interaction. Data-driven, generative models can create new datasets for multiscale models, and, conversely, multiscale modeling can provide training or test instances to create new surrogate models. Neural networks can be classified as deterministic or probabilistic.

Probabilistic neural networks go beyond single value predictions and capture the variation of real data and the uncertainty, determining the whole probability distribution. An example of a probabilistic neural network is a Gaussian process. A Gaussian process is a generalization of the Gaussian probability distribution and a particular case of the Bayesian neural network. The use of Bayesian neural network can help to identify unreliable predictions. The purpose of this type of models, that combine Bayesian inference with neural networks, is to quantify the uncertainty introduced by the models in terms of output and to explain the trustworthiness of the prediction. The weights and output of the model are statistical distribution, not unique values.

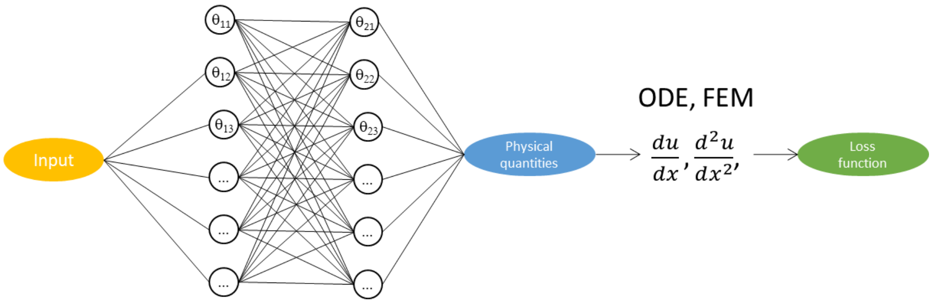


Figure 0. *– Physical informed neural network scheme.*

Data-driven models formulated with machine learning or deep learning can be viewed as an alternative to classical physics when the amount of available data is sufficient. The small data regime entails NN architectures as physics-informed neural networks, which are essentially data-efficient learning machines capable of leveraging the underlying laws of physics, expressed by time dependent and nonlinear partial differential equations, to extract patterns from high dimensional data generated from experiments.

The methodology provides a promising new direction for harnessing the long-standing developments of classical methods in applied mathematics and mathematical physics to design learning machines with the ability to operate in complex domains without requiring large quantities of data. Physics informed neural networks are intermediate tools that enhance classical numerical methods for solving partial differential equations (e.g., finite elements, spectral methods, etc.). Classical methods can coexist in harmony with deep neural networks and offer invaluable intuition in constructing structured predictive algorithms. This combination simplifies the implementation opening a potential for new possibilities in material science and data-driven scientific computing.

VALIDATION STRATEGY

A good example to validate the applicability of the methodology proposed in industrial quality control is the residual stress measurements. There are several techniques to determine residual stresses. The only non-destructive technique that can be applied in quality control to crystalline materials in an industrial environment is X-ray diffraction. However, its application in industrial environments is problematic due to some important limitations as the measurement time or non-destructive measurements below the surface: A typical residual stress measurement by laboratory X-ray diffraction in steel takes approximately 10-15 minutes per point. This is too long for in-line quality control in a production environment. The low penetration of laboratory X-rays in engineering materials – typically 15 microns in steel – means that non-destructive measurements of residuals stresses can only be performed at the component surface. This is a significant limitation, because in most fabrication processes the residual stress field – i.e., the value of residual stress vs. depth below the surface– is needed. In fact, residual stresses are already specified in several standards and in the drawings of some components, not only at the surface, but also at defined depths below the surface. Presently, the only way to measure residual stresses by diffraction below the surface in a non-destructive way involves large-scale scientific infrastructure, i.e., neutron radiation (nuclear research reactors and spallation sources) and high-energy synchrotron radiation, which is not applicable to industrial production.

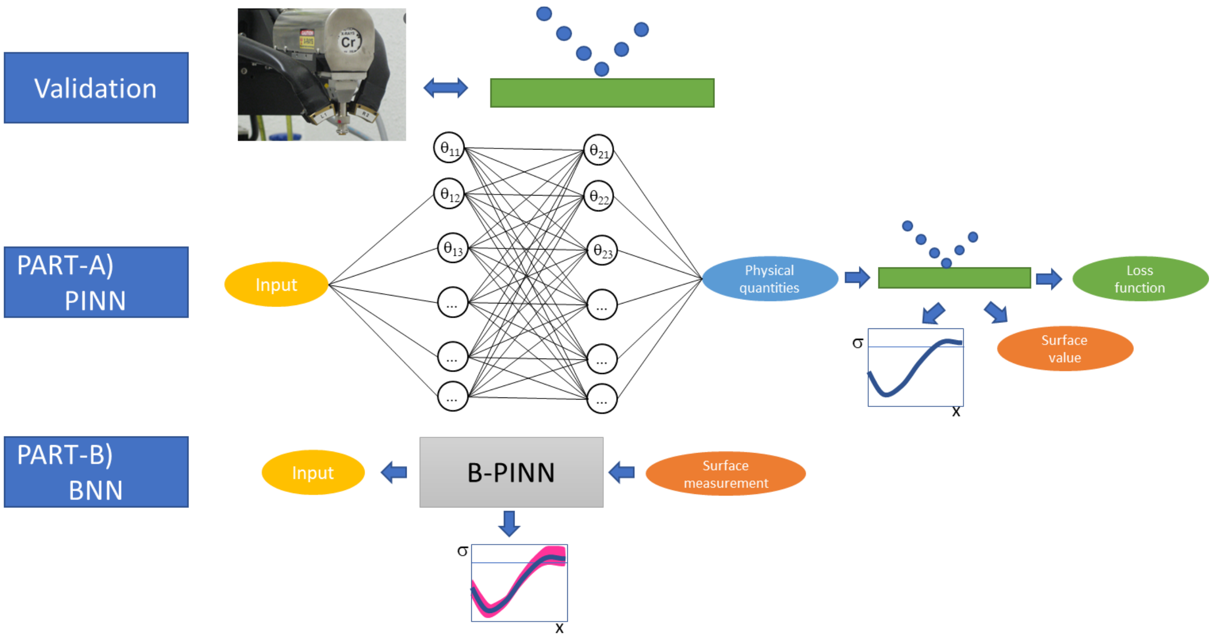


Figure 2. *– Proposed methodology application to quality control, as an example of the methodology capabilities at an industrial environment.*

The methodology proposed solves the limitations outlined above.

In aerospace and automotive industry, shot peening is the most widely used method to intentionally introduce residual stresses. The method consists of projecting small shots at high velocity over the surface of the component. The objective is to generate a compressive residual stress field below the surface –typically up to 0.5 mm depth. If the component is subjected to fatigue (as happens in many aerospace and car components), compressive residual stresses will counteract fatigue stresses and crack initiation will be slowed down, thus enhancing the component life. Consequently, the residual stress field should be known to accurately predict the fatigue life of the component. The resulting residual stress field depends on the material properties and the shot peening parameters, such as the mass, geometry and hardness of the shots, the impact velocity and the incident angle. To achieve the maximum life extension these parameters must be optimized.

An efficient method to predict the residual stress profile is finite element analysis. The models consider the impact at high velocity of a sphere or a set of spheres on the material surface and the subsequent plastic deformation, which will generate compressive residual stresses up to a certain depth. The finite element simulations will be used to amplify the information of the residual stress field measured by X-ray diffraction at the surface. The final output is the residual stress profile (in-depth) as a function of the process parameters.

The validation strategy will be divided into two parts. The first part (part A) will develop a neural network that relate the process parameters with the residual stress profile and the residual stress value at the surface. The neural network will extend the finite element simulation to the complete parameter space. The second part (part B) will formulate a Bayesian Neural Network to manage the statistical formulation. The numerical problem will be a stochastic character due to high rank of randomness of the boundary conditions. A Bayesian neural network will be introduced to model the conditional posterior distribution of the residual stress profile. The steps of the complete procedure are the following:

- **Frame the problem**: The physical and mechanical fundamental equations will define the number of features and model space. Most of the features – dimensions of the shots, angle of impact or velocity – are stochastic, with known statistical distributions. The limits of the model space will be analysed in an iterative process, checking that all variables are inside the region under study.

- **To collect, process and explore data (Part 1):** The data required for the training in part 1 will be obtained from numerical simulations. Consequently, data will be generated during the training process.

- **To perform in-depth analysis (Part 1):** A physics informed neural network will be constructed integrating NN with finite element analysis. The NN relates the process parameters with the residual stress profile and the residual stress at the surface. The proposed algorithm, PINN, will solve together the finite element simulation and the neural network fitting.

- **To collect, process and explore data (Part 2):** The second part of modelling will correlate the observable magnitude during the quality control process, the residual stress at the surface, with the process parameters.

- **To perform in-depth analysis (Part 2):** A Bayesian neural network will link the uncertainty of the observable magnitude from the quality control and the uncertainty of the process parameters, with the final distribution of the residual stress profile.

- **To communicate and apply the results:** The final output of these steps will be a neural network combination that makes use of physical laws and scatter measurements to provide and amplify the residual stress information and quantify the aleatoric uncertainty arising from the randomness of the shot peening process and the quality control measurement.

SUMMARY

The final target of our methodology is to formulate a new methodology to develop hybrid models to be applied in real time industrial applications. The new models will also be formulated in a probabilistic framework to manage the uncertainty by means of probabilistic neural networks.

REFERENCES

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