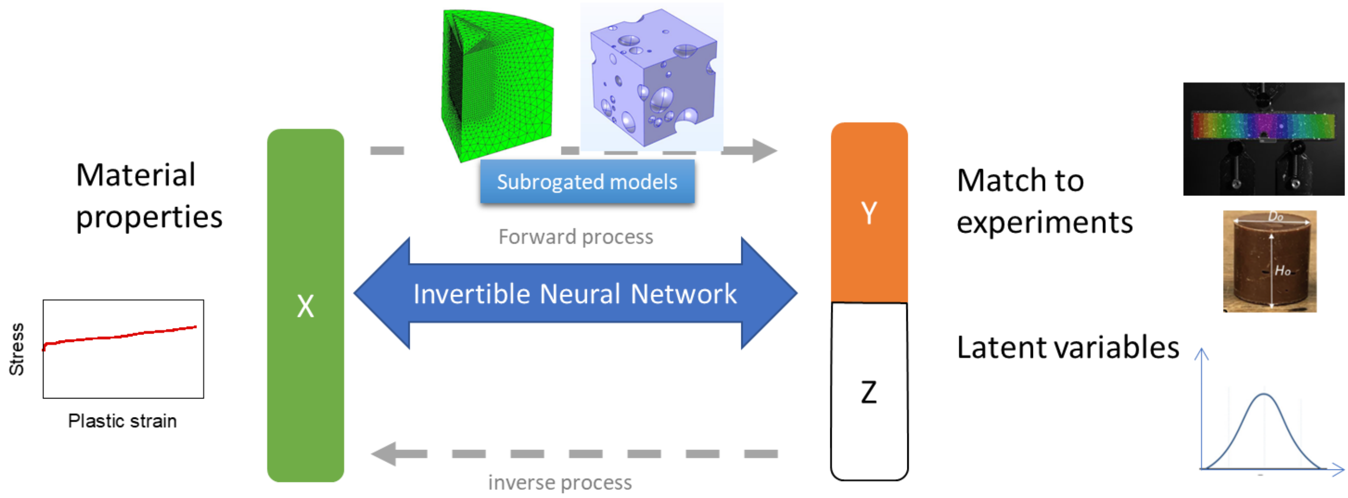
INVERSE MATERIAL CHARACTERIZATION BASED ON ARTIFICIAL INTELLIGENCE



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.

Materials science, and specifically the characterization of materials, faces significant challenges today. The development of new materials such as graphene, nanomaterials, biomaterials, hydrogels requires a deep review of the conventional characterization techniques. The heterogeneity, the anisotropy, the great variability are only some examples of the need for adaptation. The knowledge of the final properties of a component has always been a complicated task due the dependence on the manufacturing process. New forms of fabrication methods such as additive manufacturing, or new treatments, such as advanced coating, introduce complexity by generating regions with gradients, residual stresses, and general heterogeneity. The emergence of new experimental and modelling techniques tries to partially solve these drawbacks. The new developments in materials modelling, such as **Multiphysics or multiscale** analysis, are closely linked to characterization, not only because the new models require new properties, but also because they provide new methods through **inverse analysis**.

The **data-driven models** are powerful alternatives to physical modelling leveraging the innovations in Machine Learning (ML) and Deep Learning (DL). The pace of all these new developments requires a quick a holistic response, one where material characterization integrates new experimental and new modelling techniques including Multiphysics and multiscale modelling and **artificial intelligence**. Artificial intelligence (AI) is the most differentiating ingredient whose recent explosive growth must be leveraged in the development of new methods for characterizing materials.

ADVANCED MATERIAL SIMULATION company aspires to develop and validate a new and original material characterization methodology based on the combination of novel experimental techniques, advanced modelling, and artificial intelligence This new smart characterization methodologies will facilitate the design of new sustainable materials and products, and new experimental testing devices to be used with complex materials.

METHODOLOGY

Some NN architectures have been identified as potentially useful for material characterization, combining data-driven with physical laws, for example, surrogate models, Bayesian neural networks, and invertible 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

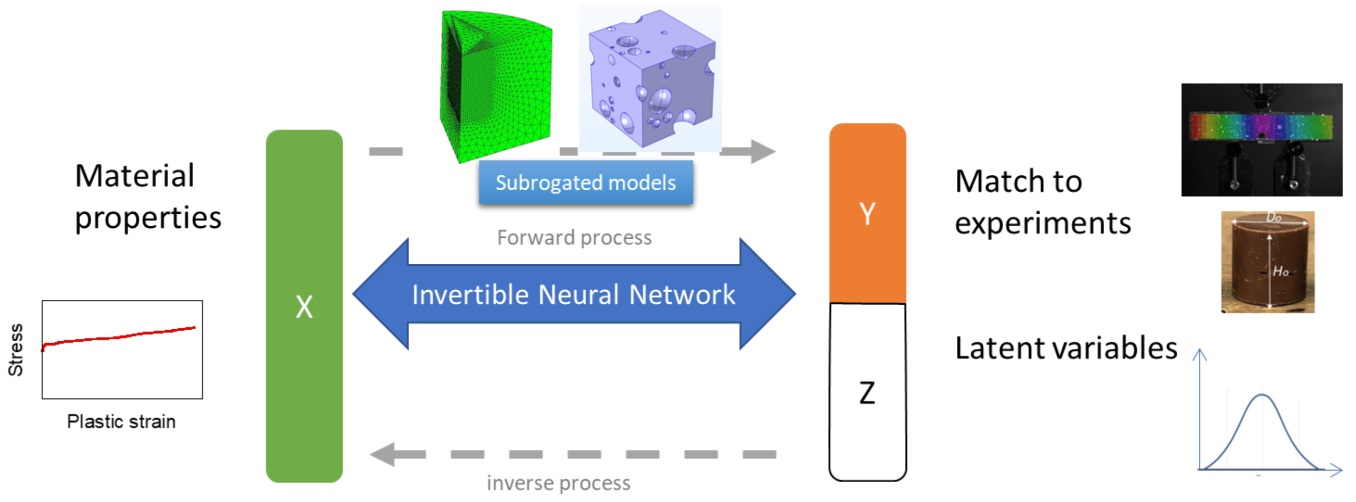


Figure 0. *- Inverse methodology proposed.*

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. 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. This type of NN can be used alone or in conjunction with invertible neural networks.

A potentially interesting NN class for this inverse problem is the **invertible neural network** (INNs). The use of probabilistic neural network and a particular class of invertible neural networks establish a proper framework to complement the inverse analysis study to determine the material properties from experimental data. This methodology has been applied successfully to determine mechanical properties as the plastic stress strain curve from nanoindentation tests or damage parameter from diametral compression tests, including the uncertainty of the results. Invertible neural networks introduce additional latent output variables to capture the information otherwise lost maintaining a biunivocal mapping. Due to invertibility, the model of the corresponding inverse process is learned implicitly. Given a specific measurement and the distribution of the latent variables, the inverse pass of the INN provides the full posterior over parameter space. The final output is the full posterior distribution for each of the materials properties, conditioned by the observed measurements, solving the ambiguity of the inverse problem.

VALIDATION STRATEGY

New materials present new challenges at the laboratory level and traditional experimental techniques must be revised and modified, as for example, in determining the mechanical properties biological materials. From a mechanical point of view, this group of materials has very complex response Continuum mechanics theories such as hyperelasticity, viscoelasticity and poroelasticity, must be applied to describe the non-linear and rate-dependent behaviour. The availability of accurate constitutive material models, that can underpin these simulations, is essential. The validation strategy will be organized in the following steps.

- **Frame the problem**: The continuum mechanics fundamental equations link the material properties that must be measured, with the observable physical magnitudes and facilitate the non-dimensional formulation. The mechanical modelling will give a holistic and integrative approach of all experimental data, framing the problem. In addition, A model space or parameter space will be defined, determining their limits iteratively, modifying them with the information obtained.

- **Collect raw data**: The raw data includes experiments and numerical simulation. The numerical simulations will model the experimental tests and will be carried out inside the model space. Apart from mechanical tests, the statistical distribution of the relevant magnitudes will be necessary for the construction of the mechanical modelling.

- **Process and explore data**: The finite element analyses carried out in step 2 above will generate raw data for data driven analyses. Due to the high computational demands of finite element models, a surrogate model will be developed. This surrogate model will map the input–output relationships of the more complex, computationally intensive finite element models.

- **Perform in-depth analysis**: The proposed solution is to apply an inverse analysis procedure that applies ML to determine the mechanical properties, which in turn better predict the experimental results; or in a probabilistic form, the materials properties that maximize the probability of obtaining the observed data. The specific neural network proposed will be an invertible neural network. This type of NN has two directions: forward direction calculating the experimental results from materials properties and inverse direction determining the materials properties from experiments. Networks that are invertible can trained on the forward process and then applied during the inverse process. The network will be trained with the numerical data to fit the parameters of the neural network and will be used in its inverse form to calculate the material properties from the experimental tests.

- **Communicate the results and the fundamental understanding**: The final result of the model will be a statistical distribution of mechanical properties that, when introduced in a numerical model, predict the experimental results. The statistical distribution of the parameters will be part of the solution to quantify the uncertainty of the procedure. This inverse problem is often ill-posed, To fully assess the diversity of possible inverse solutions for a given measurement, an inverse solver should be able to estimate the complete posterior of the parameters, conditioned on an observation. This makes it possible to reveal multi-modal distributions. The issues in framing of the inverse problem will be solved by the introduction of additional latent variables to avoid the information loss during the forward process.

SUMMARY

The final target of our methodology is to determine the set of materials models that better explain all data, including the experimental results, microscopy, numerical multiscale/multiphysics simulations with the same degree of uncertainty. The inverse problem formulated here consists of determining the material properties, and their uncertainty, which when introduced in the simulations, better predict the experimental results. The final output is the full posterior distribution for each of the materials properties, conditioned by the observed measurements, solving the ambiguity of the inverse problem.