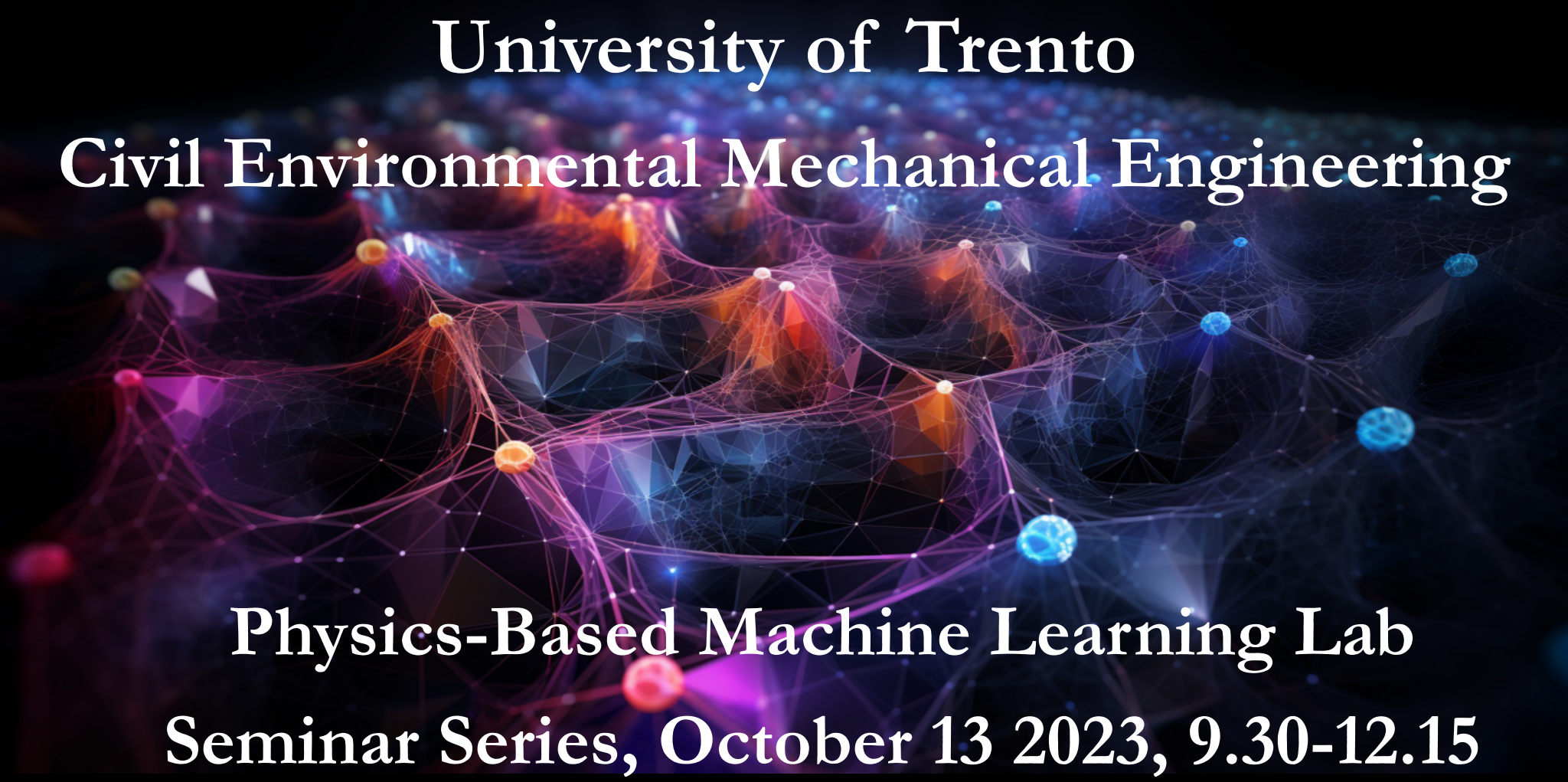
University of Trento

Civil Environmental Mechanical Engineering



Physics-Based Machine Learning Lab

Seminar Series, October 13 2023, 9.30-12.15

Aula polifunzionale BUM

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9:30 – 9:40 Director Prof. Oreste S. Bursi: Introduction of the Physics-Based Machine Learning Lab (PBMLab) as part of the Progetto Dipartimento Eccellenza 2023-27.

9:40 - 10:00 Prof. Marco Broccardo. Introduction and presentation of the Seminar series.

10:00 -11:00 Keynote: Prof. Orazio Giustolisi: *Symbolic Machine-Learning using EPR: History, Concepts and Motivation*. Polytechnic University Bari.

10:00 -11:15 Coffe break.

11:15 -11:45 Prof. Giuseppe Puglisi. *Multiscale approaches for the thermo-hygro-mechanical behavior of spider silks*. Polytechnic University Bari.

11:45 -12:15 Dott. Vincenzo Fazio. *Integrating machine learning and theoretical knowledge for new insights into multiscale phenomena*. University of Trento.

DICAM-Progetto Dipartimento Eccellenza

Dipartimento Eccellenza 2023-27

Symbolic Machine-Learning using EPR: History, Concepts & Motivation

Orazio Giustolisi
Dep. Civil, Env., Land, Build. Eng Chem., Polytechnic University Bari, Italy (orazio.giustolisi@poliba.it)

Digital transition is defined as the review of processes, using products based on digital products, technologies (hardware) and strategies (software), to increase efficiency. The simpler, more accessible, and representative collection and evaluation of data relating to processes is the knowledge base to provide useful information for efficiency. The process to be made efficient is here the scientific knowledge.

The technological event, then, does not explain and is not alone the digital transition. In fact, at the basis of today's digitalization there are always humas who developed the theories, paradigms and concepts that generated the strategies, methods, and algorithms. The scientific foundation for today's digital transition can be traced back to fields like mathematical logic and mathematics, which have evolved over centuries.

Key milestones in this journey include Alan Turing's introduction of algorithms and calculating machines in the 1930s, paving the way for computers and machine learning. The term "artificial intelligence" emerged later, but it's more appropriately described as "machine learning" or "data-driven" due to its limitations in replicating human reasoning and consciousness. The idea of artificial intelligence was born with McCulloch and Pitts in 1943 when they published a work showing a simple system of artificial neurons able to perform basic logical functions. At least in theory, this system could learn in the same way that humans learn by using experience through the trial and error that strengthens or weakens the connections between neurons. Genetic algorithms, a form of evolutionary optimization, have also contributed to process efficiency strategies. They allow for multi-objective problem-solving and are particularly suited for combinatorial problems.

We analyze some fundamental stages, which, in the past have given rise to the scientific and conditions of the digital transition and the specific symbolic machine-learning strategy, named Evolutionary Polynomial Regression (EPR). Such strategy employs genetic algorithms to search for models in data. It has its roots in John Koza's paradigm of genetic programming, which combines machine learning and evolutionary optimization. EPR focuses on symbolic modeling of data. This is a paradigm opposed to that of artificial neural networks, which are general mathematical structures characterized by the "universal" ability to interpolate data, but, for this reason, not suitable for the interpretation of the results with respect to the physical knowledge of the expert about the modeled cause-effect phenomenon. EPR-MOGA, an extension of EPR uses genetic algorithms to find models with a balance between complexity and data fitting. It seeks to strike a balance between model simplicity and data fitting in a Pareto front interpretation, enabling experts to choose the best model by considering the entire set of models and their symbolic structures, complexity, and data fitting performances. This approach supports decision-making in scientific knowledge and process efficiency.

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Abstract, second talk

Multiscale approaches for the thermo-hygro-mechanical behavior of spider silks

Giuseppe Puglisi

Dep. Civil, Env, Land, Build. Eng Chem., Polytechnic University Bari, Italy (giuseppe.puglisi@poliba.it)

Due to their extraordinary properties, spider silks represent one of the most intensively studied material, also in the spirit of biomimetics. The availability of more and more sophisticated experimental techniques let in the last decades a deeper understanding – both from a chemical and structural point of view – of the complex multiscale, hierarchical material structure at the base of their notable mechanical behavior. Nevertheless, due to the complexity of their behavior, many important phenomena regulating its loading history dependence, rate, temperature, and humidity effects, remain unclear, especially when multiscale effects are taken in consideration. We present a microstructure inspired model to deduce the macroscopic (homogenized) behavior of spider silks based on a detailed analysis of the material response at the macromolecular scale. An energetic analysis let us determine the main competing terms associated with the unfolding of beta sheets during molecule stretching and the resulting variation of the natural configuration of the molecules. Moreover, based on classical Statistical Mechanics approaches we are able to consider the fundamental effect of both temperature and humidity in the mechanical behavior of the chains. In such a way, we analytically describe the mechanical behavior of unfolding molecules, with a remarkable possibility of analytically predicting important experimental effects. Eventually, by adopting classical multiscale approaches of material modelling, we deduce the macroscopic thermo-hygro-mechanical response of the macroscopic spider silk wire, with residual stretches, hysteresis and damage directly depending on the properties of the molecules such as persistence and contour length, as well as unfolding energy of the crystal domains. The comparison with experimental tests, some of them conducted here in the Trento University (Laboratory for Bioinspired, Bionic, Nano, Meta Materials & Mechanics), reveal the effectiveness of the model in capturing the complex experimental material response considering the main dissipation and permanent strain effects depending also on temperature and humidity conditions.

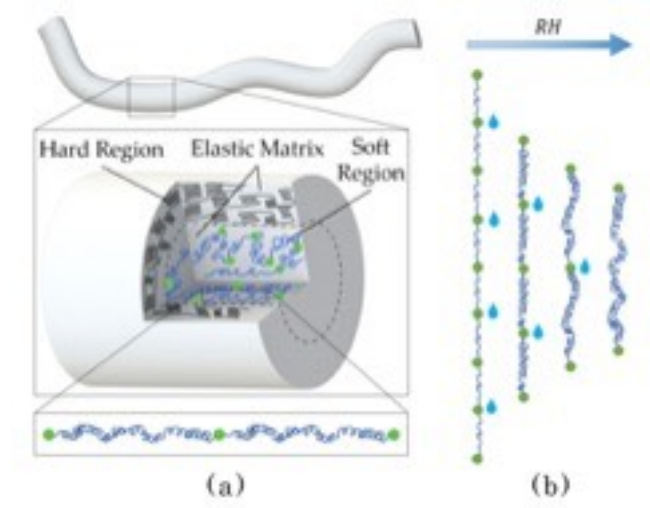

Figure 1: (a) Model of the spider silk fiber. (b) Humidity effect in the soft region.

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Integrating machine learning and theoretical knowledge for new insights into multiscale phenomena

Vincenzo Fazio

Dep. of Civil, Env. and Mech. Eng., University of Trento, Trento, Italy (vincenzo.fazio@unitn.it)

Multiscale phenomena exhibit complex structure-function relationships, and predicting their macroscopic behavior requires deducing differential equations at different scales. The complexity of these equations and the number of essential parameters make developing effective, predictive models challenging. To overcome this, researchers explore leveraging advanced numerical techniques from artificial intelligence and machine learning.Here, we focus on a fundamental aspect in multiscale phenomena, i.e. the recognition of the hierarchical role of variables. By adopting a symbolic data-driven technique based on evolutionary polynomial regression (EPR) and through a Pareto front interpretation, we aim to deduce simple and accurate relations for material modeling, starting from experimental multiscale analyses. From a physical point of view, the aim is to deduce information at higher scales from lower scales data, possibly respecting their hierarchical order. A crucial aspect of the proposed approach is the deduction of possible causality relations among the different variables to be compared with the available theoretical notions and potentially new interpretations resulting by the data modelling. This result in a stepwise approximation going from data modelling to theoretical equations and back to data modelling.To demonstrate the key advantages of our multiscale numerical approach, compared to classical, non-physically based data modelling techniques, we consider the explicit example of spider silk, known for its exceptional properties and bioinspiration potential. Indeed, it presents a complex behavior resulting from mesostructures formed by the aggregation of amino acids at the molecular scale.We argue that, due to the generality of our results, our approach may represent a proof of concept in many fields where multiscale, hierarchical differential equations regulate the observed phenomenon.

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