

**Ph.D. in Information Technology
Thesis Defenses**

May 5th, 2025

At 3:00 p.m.

Sala Conferenze Emilio Gatti – Building 20

Andres Felipe CORDOBA PACHECO – XXXVII Cycle

LEARNING-BASED OPTIMAL MANAGEMENT AND CONTROL FOR SUSTAINABLE ENERGY SYSTEMS WITH STORAGE CAPABILITIES

Supervisor: Prof. Fredy Orlando Ruiz Palacios

Abstract:

During the last decades, the world has seen a rapid change and capillary diffusion of electronic devices in every part of our life. From wearable electronics to smart devices passing through the thousands of sensors present nowadays in each new car and transportation vehicle; the amount of electronic devices around us has drastically risen.

This progress is fueled by the improvements of non-volatile memory storage capability. Each device has to have a small portion of data that should be conserved even when the system is powered off. Flash technology dominates the market in this field thanks to its reliability and scaling properties. During the last years this progress seems to have reached a halt. This is mainly due to physical reliability reasons that makes scaling the Flash memory cell a very strenuous task.

Is in this context, where large foundries are trying to develop alternative memory solutions with a high speed, large density, good scalability and reliability characteristics, that Phase Change Memory (PCM) devices have their role. These elements store the information in the atomic arrangement of the material (amorphous or crystalline) rather than the charge on a capacitor. This thesis will aim to explain and show different studies on the latest and most advanced PCM technology from STMicroelectronics; the embedded Ge-rich GST PCM.

Understanding the device physics is fundamental to predict and control the element behavior. In order to do this thorough analysis of electrical data was complemented with physical images such as Scanning Transition Electron Microscopy (STEM) or Electron Energy Loss Spectroscopy (EELS) to support the evidences. These data were used to create physics based modeling framework able to predict both electrical and physical evidences. The models shown range from a relatively simple analytical models to three dimensional thermo-electrical Technology Aided Computer Design (TCAD). Different tools for simulations were used from Comsol Multiphysics to the Synopsis Sentaurus suit passing through the development of some modules of Ginestra, the Applied Materials proprietary simulation software.

The device behaviors covered in this work permeate the memory life from production to application. The peculiar Ge-rich GST material evolution of the cells from process deposition to programming is shown considering both phase and composition. Time evolution of resistance level in the phenomena called drift with the complex temperature dependence and relation with crystallization. Applications of these devices to possible revolutionary new field such as Analog In-Memory Computing and evaluation of their perspective performances. This work is a product of the excellent collaboration between Politecnico di Milano and STMicroelectronics, in particular the Agrate PCM Excellence Center lead by Roberto Annunziata, that provided the data related to PCM devices.

Marco LEONESIO – XXXVI Cycle

**PHYSICS-ENHANCED MACHINE LEARNING METHODS FOR INDUSTRIAL
PROCESS MODELING AND OPTIMIZATION**

Supervisor: Prof. Lorenzo Mario Fagiano

Abstract:

The recent and significant developments in the field of digital technologies and Artificial Intelligence (AI) suggest their pervasive application even in the sector of capital goods and production systems. In particular, enablers such as smart sensors with local intelligence, machine networking, data mining techniques, and machine learning support the development of "Intelligent Machines". These will provide services in terms of production process monitoring, parameter optimization, and collaborative interaction with the operator, making them more autonomous, flexible, and efficient. This perspective is part of a well-defined National and European strategy that sees AI as one of the main tools for implementing the so-called Industry 4.0 Transition of production systems (PNRR). On the other side, according to the newer paradigm of Industry 5.0, Intelligent Machines are expected to be not only sustainable and resilient, but also "human-centric". Regarding this latter characteristic, we think there is ample room for developing automation approaches that involve sharing knowledge and control capabilities between the operator (more or less experienced) and the Intelligent Machine. This sharing is facilitated through a series of enabling technologies related to the world of AI.

On these premises, this thesis is focused on modeling and optimization approaches for industrial processes that try to combine the generality and extrapolative capability of first-principle models (including the domain knowledge of experts) with the adaptive capabilities of data-driven methods, typical of machine learning. This would allow for achieving acceptable levels of accuracy even with limited data availability. These approaches can be framed in the paradigm of physics-informed, or physics-enhanced AI.

Investigating Random Forest as a promising machine learning method suited to generate surrogate models in the case of small datasets, the problem of the global optimization of an objective function represented by this kind of model came to our attention. In particular, an original method to obtain an approximate global minimum at low computational complexity has been developed, resorting to the inherent structure of a Random Forest, which is traceable to a non-parametric model that partitions the feature space in convex orthotopes by applying binary splits on training data. Our approximate method shows optimality performances that are comparable to other exact approaches based on the solution of a Mixed Integer Linear Program, which entails a combinatorial complexity and cannot be applied to a large Random Forest operating in a high-dimensional feature space (curse of dimensionality).

Then, seeking a way to increase the accuracy of the model in predicting the production quality class, a novel physics-informed learning approach for this problem is proposed. The approach relies on a hierarchical semi-supervised classification, where the training data, classified on the basis of the three quality intervals of interest, are divided in a certain number of sub-clusters with respect to the process input parameters (primary features) and enhanced with the classification prediction provided by a physics-based model (apriori knowledge injection).

To evaluate the effectiveness of the above-mentioned methodological achievements in the context of a real manufacturing setting, the centerless grinding production process has been considered. In the absence of proper experimental data, a high-fidelity model has been developed to generate a synthetic dataset, which is augmented with the predictions of a low-fidelity model representing the apriori physics-based knowledge about the process. The resulting dataset has been used both to grow a Random Forest and optimize its output, as well as to test the performance of the proposed Semi-

supervised physics-informed classifier. Other state-of-the-art approaches to generating gray-box models have been evaluated, mostly based on Feed Forward Neural Networks.

The results show the effectiveness of the proposed random forest optimization approach and quality classifier, especially dealing with a high-dimensional variable space. On the other side, the overall absolute performance of the hybrid models, in comparison with the pure data-driven counterpart, suffers from the smallness of the considered dataset with respect to the target behavioral complexity: the first principle predictions are not accurate enough to compensate for the lack of data.

PhD Committee

Prof. Francesco Casella, **Politecnico di Milano**

Prof. Moschos Papananias, **Brunel University London**

Prof. Carlos Ocampo-Martinez, **Universitat Politecnica de Catalunya**