

DEPARTAMENTO DE CONTROL AUTOMÁTICO

Dear Professor Paolo Carloni,

We propose the following project within the framework of the collaboration between the Centro de Investigación y de Estudios Avanzados of the Instituto Politécnico Nacional and the Jülich Research Center.

***Exploration of the Attractor Landscape in Gene Regulatory Networks Associated with the Emergence and Progression of Chronic Degenerative Diseases Using Quantum Computing***

**Background**

Researchers from the Department of Automatic Control at Cinvestav, in collaboration with national and international partners, develop models of gene regulatory networks (GRN's) based on curated experimental genomic data. These models address mechanisms involved in the emergence and progression of chronic degenerative diseases, including epithelial cancer, metabolic syndrome, and colon cancer. Several networks have been characterized whose dynamical attractors correspond to clinically relevant phenotypes. Exploration of attractor landscapes—crucial for identifying therapeutic intervention strategies—typically relies on brute-force simulations of discrete Boolean networks describing gene regulatory interactions. However, these methods scale poorly due to the combinatorial complexity of the state space. Examples include networks associated with epithelial-to-mesenchymal transition in epithelial cancer [1], hepatic cancer stem-cell dynamics [2], and transcriptional regulation of the cell cycle [3]. Such networks often involve an important number of nodes, making exhaustive computational exploration challenging. At the same time, advances in single-cell sequencing technologies, particularly RNA-seq, have greatly increased the volume and resolution of transcriptomic data. This development highlights the need for new computational approaches capable of exploring attractor landscapes in large GRN's, a key challenge for precision medicine.

**Project**

Recent studies have proposed the use of quantum computing both for inferring gene regulatory networks from single-cell transcriptomic data and for exploring their attractor landscapes. The objective of this project is to evaluate quantum computing methods for exploring the attractor landscapes of medium-scale gene regulatory networks. The study will focus on regulatory networks associated with loss of cellular identity in epithelial cancers, considering the effects of tumor dynamics on cell-cycle regulation and the formation of the tumor microenvironment, including the adaptive response of the immune system. We will investigate algorithms designed to infer logical relationships among genes from single-cell RNA-seq data, including the qubit-entanglement approach for simulating gene interactions [4]. In addition, we will explore algorithms for attractor landscape characterization, such as the quantum amplitude suppression method [5]. These methods will be implemented as hybrid classical-quantum algorithms compatible with the computational infrastructure available at the Jülich Research Center. Applications will prioritize colon and hepatic cancer, while adapting Boolean-network modeling approaches that incorporate Cartesian visualization techniques [6].

**Participants**

Dr. Juan Carlos Martínez García (Professor-Researcher, Technical Lead); Dr. Moise Bonilla Licea (Postdoctoral Researcher); Dr. Moisés Bonilla Estrada (Professor-Researcher); Dr. Alberto Soria López (Professor-Researcher); Dr. Antonio Bensussen (Investigador por México – Secihti); M.Sc. Jesus Nazario Piñon Meza (Doctoral Student)

**References**

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Best regards,

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