# Q DAYS

# 11 - 12 April 2019

## ABSTRACTS

### **INVITED TALKS**

Ricardo Ribeiro (CFUM) The quantum paradigm

Abstract: If the first quantum revolution implied a change of paradigm relative to classical mechanics, the second quantum revolution that we are experiencing takes the new paradigm to its full consequences. In this talk, the main features of the quantum paradigm are reviewed, with an emphasis on the technologial implications.

Rui Soares Barbosa (DCS, Oxford) Quantum vs classical: non-locality, contextuality, and informatics advantage

Abstract: This talk is an introduction to the study of some of the characteristic observable features of quantum systems that distinguish them from classical systems. In particular, we will focus on the concepts of non-locality and contextually with an emphasis on their role as resources that provide quantum advantage in computational and information-processing tasks.

### **TUTORIALS**

Local researchers present the fundamentals of quantum computing.

### HANDS-ON-SESSION: IBM Quantum Experience

Afonso Rodrigues (HASLab) and Ana Neri (HASLab)

Learn more about quantum computing on the cloud with the IBM Q Experience and a hands-on session with QISKit, a quantum software toolkit for the development and study of quantum algorithms and their applications. The session will include a brief introduction to the software and properties of state-of-the-art quantum devices, and demonstrate the implementation and execution of quantum algorithms. <u>PLEASE BRING YOUR LAPTOP.</u>

### POST-GRADUATE STUDENTS SESSION

#### S. Di Giorgio (IST & IT)

Quantum Markov networks: recoverability of quantum states from direct correlations

Abstract: Graphical models are widely used techniques for inferring the most likely probability distribution that describes a system of classical random variables. The structure of the graph encodes conditional independence properties between the variables, that results in a factorization of the maximum entropy estimator, the more non-committal one with regard with missing information. Quantum states are completely described by density operators on a Hilbert space. When the number of degrees of freedom increases, the resources needed to infer the state become computationally demanding. Since density operators encompass probability distributions, naturally arise the question of whether it is possile to define a generalized graphical model that encodes quantum states and correlations, and graph techniques for learning quantum systems. Quantum Markov networks are preliminary models.

Starting from the easiest but non-trivial quantum network, tripartite scenario when two out of three direct correlations between the subparts are known, I explore the notion of quantum conditional independence. I define quantum Markov chain and see the connection with the maximum entropy estimator, providing an algebraic necessary and sufficient condition for the desired estimator to be efficiently inferred from the given set of marginals. The developed procedure reduced Bayes rule or Hammersley-Clifford theorem when the information encoded in the density operator is purely classical. Moreover, I provide a characterization of the procedure in light of the Quantum Bayesian updating. I am going then to generalize the technique to the multipartite scenario, restricting to quantum states which associate graph is a tree.

Carlos Tavares (HASLab) Quantum simulation

Abstract. As quantum computing finally comes of age, with its first commercial implementations, quantum simulation emerges as a ground- breaking technology for several domains, including biology and chemistry. Nonetheless, the process of building quantum simulations can be non-trivial, raising a number of conceptual and practical challenges at different levels, from the conception to its actual execution. We go through such challenges, in a case study of a quantum simulation for the hydrogen (H2) and Lithium-hydride (LiH) molecules, in an actual commercially available quantum computer, the IBM Q, while opening prospects to new simulations on similar regimes.

#### Bruno Murta (INL)

Tackling the Many-Body Problem with Noisy, Intermediate-Scale Quantum Computers

Abstract: Conventional numerical methods to describe quantum many-body phenomena face the so-called exponential wall problem: the computational resources scale exponentially with the number of degrees of freedom. Classical simulations have thus failed to address strong interactions, for which approximations such as perturbation theory or Density Functional Theory have intrinsic limitations, and two- and three-dimensional problems, for which Density Matrix Renormalization Group and tensor networks are of little use with classical hardware. Quantum simulation via

quantum computing arises as a natural alternative by taking advantage of quantum parallelism. In this talk I shall give an outline of digital quantum simulation strategies, including adiabatic evolution, exact quantum algorithms, and hybrid variational methods. I shall discuss the limits of current state-of-the-art quantum hardware to simulate quantum systems and identify condensed matter systems where digital quantum simulations will eventually outperform classical numerical simulations.

## Carolina Alves (HASLab) QGraphics: quantum searching for ray triangle intersection

Abstract: The main focus of this work is to apply the Grover's Algorithm (a quantum search algorithm) to computer graphics problems. One of the most used algorithms in the computer graphics field is ray tracing. This technique allows computing visibility between 2 points in a 3D model of the world which is described by a collection of geometric primitives (e.g., triangles). The algorithm returns, for a given ray, which triangle it intersects closest to its origin. Grover's Algorithm is a quantum search algorithm based on amplitude amplification that provides a quadratic speed up allowing visibility evaluation in  $O(\sqrt{N})$  evaluations of the function for unstructured scenes. Since ray tracing can be a very computationally demanding task the goal is to develop a quantum ray tracer using Grover's algorithm benefiting from the time advantage in computation that it provides.

## Michael Oliveira (HASLab) Quantum Bayesian inference

Abstract: As a compact representation of joint probability distributions over a dependence graph of random variables and a tool for modeling and reasoning in the presence of uncertainty, Bayesian networks are becoming increasingly relevant both for natural and social sciences, for example, to combine domain knowledge, capture causal relationships, or learn from incomplete datasets. Known as an NP-hard problem in a classical setting, Bayesian inference to support decision making pops up as a class of algorithms worth to explore in a quantum framework. This presentation explores such a research direction and improves on previous proposals by a judicious use of the utility function in an entangled configuration. A prototype implementation in QISKit (a Pythonbased program development kit for the IBM Q machine) is discussed as a proof-of-concept. Additionally, the computational complexity of the process will be analyzed.

## Daniel Carvalho (HASLab) Exploring quantamorphisms

Abstract: Up until this moment, the usual approach in the design of quantum programming languages is based on the paradigm of "quantum data, classical control", where the data may be in a quantum superposition but the flow of execution is controlled classically. The main goal of this presentation will be exploring the concept of "quantum control", which allows for the superposition of finitely many quantum operations without the need for measurements. In this context, it will also be presented a notion of quantum recursion where the recursive procedure calls will be executed in superposition.

Vitor Fernandes (HASLab)

Integration of quantum processes in cyber-physical systems

Abstract: Process algebras are standard tools for the specification and analysis of concurrent systems, whose success in applications to classic models of computation lead to a flurry of research devoted to transporting the theory to the quantum case. In this talk I will give an outline of this research: more specifically, I will present the main features of quantum process algebras, illustrate their main applications, and point out some of their limitations in timed environments.

## Sofia Oliveira (HASLab) Flexible molecular alignment

Abstract: Flexible molecular alignment is a complex problem in the area of Medicinal Chemistry where, even nowadays, the approach to nd the solution is not a certainty but, instead, a probability. The current approach to this problem is probabilistic because it does not test all possible alignments, but makes an analysis of all the variables and only 'touch' the ones with potential greater impact in the posterior alignment. This procedure can lead to wrong 'best alignments'. Quantum computation, due to his natural parallelism, may improve algorithmic solutions for this kind of problems because it may test and/or simulate all possible solutions in an execution cycle. Due to its complexity we have reduced the problem to a dozen of active properties per molecule, revisited the classical solution and start to gure out the quantum corresponding solution.