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Engineering Quantum Computing Technologies: from Compact Modelling to Applications

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Quantum computing could impact Society and Industry in an unprecedented way, especially in critical domains, such as optimization problem solving, computational chemistry and artificial intelligence. Properties of quantum mechanics, such as superposition and entanglement, can be exploited to define problem-specific quantum algorithms with lower computational complexity than their best corresponding classical counterparts. A common limitation of quantum computers is the presence of hardware non-idealities, such as decoherence, dramatically affecting performance and reliability. In any case, efforts in improving hardware and investigating short and long-term quantum algorithms can be already done.

The goal of this doctorate thesis is to explore different levels of quantum computing engineering, from devices to applications. In particular, the attention was focused on two activities: the definition of a compact-model-based simulation methodology for quantum technologies for the general-purpose quantum circuit model and the proposal of an approach for solving the users scheduling optimization problem in Joint-Transmission-based wireless communication systems, exploiting the quantum-compliant Quadratic Unconstrained Binary Optimization (QUBO) formalism.

Classical simulation of quantum computers allows a preliminary estimation of their capabilities in specific applications. Canonical simulation of qubits affected by non-ideality phenomena requires solving the computationally expensive Lindblad master equation. A compact model of a quantum technology, obtained through fitting operations or specific mimic algorithms, is thought to describe qubits evolution under quantum gates, taking into account the device-characteristic physical parameters and not numerically solving Lindblad equation, thus permitting faster and more scalable simulations. Compact models of two families of spin-based molecular quantum computers, switch-based and Nuclear Magnetic Resonance, were developed, both involving two other general non-ideality models: decoherence and off-resonance of untargeted qubits. A quantum circuits simulator, involving all these compact model approximations were compared with either results already available in the state of art or through numerical simulations with consolidated formalisms, at both Hamiltonian and circuit levels. The achieved results give evidence that the proposed simulation methodology provides results fast and close to the references, thus paving the way for fast and reliable technology-dependent quantum circuits simulation.

Joint Transmission (JT) is a modern protocol for Multiple-Input-Multiple-Output (MIMO) wireless communication systems, where multiple antennas co-operate to transmit signals to users with minimized interference. An optimization problem, looking for the best users subset servable in JT, can be defined. In a practical scenario, this cannot be efficiently solved with a *brute-force*-only approach, since it could imply a too high number of combinations. This thesis presents a strategy for solving the JT optimization problem, based on a QUBO model, which is responsible of a first selection of users among all available. The subset selected with QUBO is then *brute-force* explored, to find the best solution. In all executed tests, the obtained results permit to say that the proposed method achieves a quite good compromise between solution quality and total execution time.

Even though the obtained results in both contexts can still be further expanded and improved, they are quite encouraging and prove that these research activities, if continued in the future, can help in improving quantum computing engineering, at both hardware and software levels, with the hope that it can concretely solve problems of interest for Society and Industry.