Propuesta TFG. Curso 2025/2026

GRADO: Grado en Física

CÓDIGO DEL TFG: 267-326-2025/2026

1. DATOS BÁSICOS DEL TFG:

Título: Simulación de circuitos cuánticos y computación de alto rendimiento en clústeres heterogéneos

Descripción general (resumen y metodología):

The simulation of quantum systems is a computationally expensive problem that requires high performance computing systems. This problem is of importance in several branches of physics, traditional, such as condensed matter, but also in novel areas such as quantum computing. For example, developing classical quantum circuit simulators is important for testing and evaluating quantum technologies.

This thesis project will study how to simulate quantum circuits (the ones used in quantum computer algorithms) on supercomputers. A comparative study of different strategies to simulate quantum circuits of interest will be performed. The suitability of tools of interest to available High Performance Computing (HPC) architectures will be studied, such as, e.g., the Proteus computer of the University of Granada will be studied https://proteus.ugr.es/, or other public or private HPC centers. State of the art HPC systems consist of heterogeneous environments, comprising multiple nodes with a diverse variety of specialized processors, including multi-CPUs, and hardware accelerators such as GPUs and FPGAs. Furthermore, several of the public clusters available in Spain have recently installed Quantum Processing Units (QPU), allowing for hybrid quantum-classical computing systems to be developed.

Methodology:

Literature will be reviewed with different quantum circuit simulation strategies for heterogeneous HPC systems.

Common programming languages for optimization tasks in computational physics, such as C/C++, Python or Julia, will be used.

Existing quantum software libraries such as IBM QisKit or Microsoft Azure can be used.

Simulations will be carried out on the Proteus supercomputer of the UGR.

The performance of the simulations, cost of computational resources, memory, computing time, etc., will be analyzed.

Tipología: Estudio de casos, teóricos o prácticos, relacionados con la temática del Grado.

Objetivos planteados:

Objectives:

We will study the implementation of an advanced simulation method for quantum circuits, in such an environment. We will investigate state-of-art classical simulation methods, such as, e.g. matrix multiplication, tensor networks, convex optimization, Wigner functions, the covariant matrix formalism, symplectic geometry, stabilizer formalism, stabilizer rank methods, circuit-knitting, circuit cutting.

We will identify what type of computing hardware is optimal for physically relevant problem instances. We will focus in developing new computational physics methods for optimizing computer simulations in heterogeneous nodes, such as, available multi-node multi-CPUs, GPUS, FPGAs, which are currently available in the Proteus cluster, as well as QPUs, available in Spain in CESGA and BSC.

We will optimize the method using modern quantum information techniques, algorithmics, numerical computational physics methods and High Performance Computing paradigms.

Emphasis will be placed on the optimization of high-performance simulation tasks. Optimizations to achieve resource savings will be studied, such as, existing symmetries or linear dependencies, or mathematical structures. We will pay attention to the memory cost, time cost, energy efficiency, parallelization capacity.

A simulation of a quantum algorithm of interest for a computational problem will be implemented on a supercomputer. If access to a quantum computer is available, a hybrid quantum-classical quantum algorithm implementation will be attempted. The goal is to implement the proposed method in a heterogeneous HPC setup and obtain numerical benchmarks to gain quantitative and qualitative understanding of how modern HPCs can simulate quantum computers.

Bibliografía básica:

Andor Menczer, Örs Legeza, Massively Parallel Tensor Network State Algorithms on Hybrid CPU-GPU Based Architectures, https://arxiv.org/abs/2305.05581

Ang Li, Omer Subasi, Xiu Yang, Sriram Krishnamoorthy, Density matrix quantum circuit simulation via the BSP machine on modern GPU clusters, SC '20: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, https://github.com/pnnl/DM-Sim/blob/master/doc/paper_sc20.pdf

Daniel Strano, Benn Bollay, Aryan Blaauw, Nathan Shammah, William J. Zeng, Andrea Mari, Exact and approximate simulation of large quantum circuits on a single GPU, https://arxiv.org/abs/2304.14969

Jun Doi , Hitomi Takahashi , Rudy Raymond , Takashi Imamichi , Hiroshi Horii Authors Info & Claims, Quantum computing simulator on a heterogenous HPC system, CF '19: Proceedings of the 16th ACM International Conference on Computing FrontiersApril 2019 https://dl.acm.org/doi/10.1145/3310273.3323053

Honghui Shang, Li Shen, Yi Fan, Zhiqian Xu, Chu Guo, Jie Liu, Wenhao Zhou, Huan Ma, Rongfen Lin, Yuling Yang, Fang Li, Zhuoya Wang, Yunquan Zhang, Zhenyu Li, Large-Scale Simulation of Quantum Computational Chemistry on a New Sunway Supercomputer, https://arxiv.org/pdf/2207.03711.pdf

Salvatore Mandrà, Jeffrey Marshall, Eleanor G. Rieffel, Rupak Biswas, HybridQ: A Hybrid Simulator for Quantum Circuits, 2021 IEEE/ACM Second International Workshop on Quantum Computing Software (QCS), https://arxiv.org/abs/2111.06868

Stavros Efthymiou, Marco Lazzarin, Andrea Pasquale, and Stefano Carrazza, Quantum simulation with just-in-time compilation, Quantum 6, 814 (2022), https://arxiv.org/pdf/2203.08826.pdf.

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A. Kissinger and J. van de Wetering, 'Simulating quantum circuits with ZX-calculus reduced stabiliser decompositions', Quantum Sci. Technol. 7 044001, 2022. doi:10.1088/2058-9565/ac5d20

M. Sutcliffe and A. Kissinger, 'Procedurally Optimised ZX-Diagram Cutting for Efficient T-Decomposition in Classical Simulation', Electron. Proc. Theor. Comput. Sci., vol. 406, pp. 63-78, 2024. doi:10.4204/EPTCS.406.3

T. Carette, D. Horsman, and S. Perdrix, 'SZX-Calculus: Scalable Graphical Quantum Reasoning', in DROPS-IDN/v2/document/10.4230/LIPIcs.MFCS.2019.55, Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2019. doi:10.4230/LIPIcs.MFCS.2019.55.

J. Huang, S. M. Li, L. Yeh, A. Kissinger, M. Mosca, and M. Vasmer, 'Graphical CSS Code Transformation Using ZX Calculus', Electron. Proc. Theor. Comput. Sci., vol. 384, pp. 1–19, Aug.

2023, doi:10.4204/EPTCS.384.1.

Recomendaciones y orientaciones para el estudiante:

Es recomendable tener conocimientos previos o alto interés en física computacional, física cuántica y computación cuántica.

Plazas: 1

2. DATOS DEL TUTOR/A:

Nombre y apellidos: JARA JUANA BERMEJO VEGA

Ámbito de conocimiento/Departamento: FÍSICA DE LA MATERIA CONDENSADA

Correo electrónico: jbermejovega@ugr.es

3. COTUTOR/A DE LA UGR (en su caso):

Nombre y apellidos:

Ámbito de conocimiento/Departamento:

Correo electrónico:

4. COTUTOR/A EXTERNO/A (en su caso):

Nombre y apellidos:

Correo electrónico:

Nombre de la empresa o institución:

Dirección postal:

Puesto del tutor en la empresa o institución:

Centro de convenio Externo:

5. DATOS DEL ESTUDIANTE:

Nombre y apellidos: Marina Benítez Sánchez

Correo electrónico: mbenitez31@correo.ugr.es