Projects for ETSIST Incoming Students - PROJECT PROPOSAL

Academic year 2024 / 2025

Project description	
Project name: Extension to quantum to add support to HDF5	
Academic year: 2024/25	Semester: ◯ Fall ● Spring
Starting date[1]: 01/02/2025	Ending date[2]: 07/06/2025
UPM Centre: ETSIST	Hours per week: 7,5
Total hours: 135	Credits: 4,5 ECTS
Supervisor data:	
Name: Rafael Delgado López	
Department: matemática aplicada a las tecnologías de la información y las comunicaciones	
E-mail: rafael.delgado@upm.es	Phone: +34 9106 73461

Project contents and requisite skills

The student will contribute a GPL project (quantumfdtd). Such a code can use several techniques (finite differences and Fast Fourier Transform) to solve the Schrödinger Equation in imaginary time for an arbitrary 3d potential. It is implemented in C and Python, and uses the MPI (Message Passing Interface) standard.

Currently, the in/out of the program is CSV files. Some scripts compress and decompress them via gzip. The goal of the student will be implementing HDF5 for data management, both on the C core and on the Python analysis libraries.

The project is available in github: https://github.com/quantumfdtd/quantumfdtd_v3

Expected learning outcomes

The student is expected to contribute a GPL project. This will allow him to improve his skills in: usage of GNU/Linux systems, git system, coding in C / Python / Bash, data storage systems, MPI systems, data analysis, benchmarking,…

The project quantumfdtd is an international one involving Prof. Michael Strickland (Kent State University, USA), Dr. Johanes H. Weber (Humboldt University of Berlin, Germany), Dr. Rafael L. Delgado and former PhD student Sebastian Steinbeißer (Technical University of Munich TUM, Germany). The final goal is releasing a new version of the code with HDF5 support and a publication about it. This involves sending and defending a “pull request” to the project and the necessary international coordination in order to release a new version of the code and writing a publication.

1 Note that the starting date cannot be before the beginning of the lectures in the corresponding semester
2 Note that the ending date cannot be after the last exam in the corresponding semester

Rules for students
a) To join the project, to follow the rules and schedule agreed with the supervisor, and to duly justify any possible absence. b) To carry out the activities specified in the project schedule and to keep the necessary contact with the supervisor. c) To inform to the Internship Coordinator at ETSIST, or to the Mobility Office, of any event or complaint that may arise in the development of the project. d) To send to the Internship Coordinator at ETSIST an interim report (Annex II), a final report of the work carried out (Annex III) and the satisfaction questionnaire of the internships, according to the forms and the deadlines set in the annexes of this regulation. e) To maintain the confidentiality of the internal information of ETSIST, Department or Center to which they have got access, as well as to not exploit the work carried out in the project without express authorization.