Q@TN - *Quantum Science and Technology in Trento*

APPLICATION FORM

for PhD or postdoctoral fellowship

1. Project title: Machine Learning techniques FOR Quantum Gate Engineering (ML Q-FORGE)
2. Keywords: control theory, quantum gate engineering, circuit QED

3. Type of position requested:
- ✓ Ph.D. student
- ☐ Postdoc
- ☐ Senior postdoc

4. Duration of the position: three years

5. Estimated full cost: Euro 77,783.83 (cost of a Ph.D. fellowship as of the last deliberation of the University of Trento, Euro 67,780.13, plus 1 year of increment for periods spent abroad, Euro 10,003.69)

6. Managing partner / doctoral school:
- ☐ FBK
- ☐ UniTN
- ☐ CNR
- ✓ Doctoral School: Doctoral School in Physics

7. Proponents

prof. **Francesco Pederiva**
Associate professor, nuclear and subnuclear physics
Physics Department, University of Trento

Recent and ongoing projects:

- ANuPC-QS: Accelerating Nuclear Physics Calculation with Quantum Processing, Q@Tn project 2018.
- 2016-present: PI of the INFN national research project (Iniziativa Specifica) MANYBODY, including nodes at Trento, Rome “La Sapienza”, Bologna, Turin, Pavia, Bologna, Lecce.
- 2010-2015: co-director of LISC (Interdisciplinary Laboratory of Computational Science), a joint venture of FBK (the Bruno Kessler Foundation) and the University of Trento

Excerpt of publications:

1. Carlson, Jonathan Carter, Gandolfi, S., Pederiva, F., Pieper, Steven C., Schiavilla, R.,Schmidt, K. E., Wiringa, R. B. (2015). Quantum Monte Carlo methods for nuclear physics. REVIEWS OF MODERN PHYSICS, vol. 87, p. 1067-1118
2. Lonardoni, Diego, Lovato, Alessandro, Gandolfi, Stefano, Pederiva, Francesco (2015). Hyperon puzzle: Hints from Quantum Monte Carlo calculations. PHYSICAL REVIEW LETTERS, 114, 092301
3. Barnea, N., Contessi, L., Gazit, D., Pederiva, Francesco, Van Kolck, U. (2015), Effective field theory for lattice nuclei. PHYSICAL REVIEW LETTERS, vol. 114, 052501
4. M. H. Kalos, F. Pederiva (2000). Exact Monte Carlo method for continuum fermion systems. PHYSICAL REVIEW LETTERS, vol. 85, p. 3547-3550

5. Madeira L., Lovato A., Pederiva F., Schmidt K.E. (2018), Quantum Monte Carlo formalism for dynamical pions and nucleons, PHYSICAL REVIEW C, vol. 98, 034005

Total publications: 123. Total citations > 2117. H-index: 26 (according to Scopus on Mar. 26. 2019).
Full CV attached.

Dr. **Simone Taioli**
Senior Researcher, FBK-ECT*, Trento.

Research interests

Use of state-of-the-art and development of novel theoretical and computational methods for the first principles solution of the many-body problem in atoms, molecules, and solids at different length and time scales. The full CV in attachment.

Recent and on-going projects:

- ARTIQS: "ARTificial Intelligence for Quantum Systems"(May 2019 - ongoing) - postdoctoral call of the Q@TN consortium - total budget 160k €
- MaDEleNA: "Developing and studying novel intelligent nanomaterials and devices towards adaptive electronics and neuroscience applications" (Dec 2010 - Dec 2015) - Grandi Progetti PAT - total budget 1500k €
- 2SuperB: "Epitaxial growth of graphene and SiC layers on inorganic surfaces: a joint theoretical and experimental approach" (Jan. 2010 - Dec 2010) - FP7 Marie Curie Outgoing Researcher - total budget 30k €
- MISTICO: "New Technologies and Microsystems for solar energy cogeneration solutions¨ (March 2011- Feb 2013) - Caritro Foundation- total budget 120k €
- NEMESYS: "Non equilibrium dynamics models and excited state properties" (Nov 2016 - ongoing) - INFN strategic project - total budget 300k €
- INTELBIOMAT: Interdisciplinary Approaches to Functional Electronic and Biological Materials (April 2012 - July 2012) - European Science Foundation - total budget 6 k€
- SCIENCE FOR PEACE: "Electron energy loss techniques" in collaboration with Kurchatov Institute (Jan 2011 - Dec 2013) - NATO Collaborative Grant - total budget 20k €

5 publications relevant to the project:

- Relativistic Theory and Ab Initio Simulations of Electroweak Decay Spectra in Medium-Heavy Nuclei and of Atomic and Molecular Electronic Structure, Tommaso Morresi, Simone Taioli, Stefano Simonucci, Advanced Theory and Simulations 1800086, 1-24 (2018), JOURNAL COVER (https://onlinelibrary.wiley.com/doi/abs/10.1002/adts.201870030)
- The effects of a revised 7Be e--capture rate on solar neutrino fluxes, Diego Vescovi, Luciano Piersanti, Sergio Cristallo, Maurizio Busso, Francesco Vissani, Sara Palmerini, Stefano Simonucci, Simone Taioli Astronomy & Astrophysics A126, 7 (2019)
- Secondary electron emission and yield spectra of metals from Monte Carlo simulations and experiments,Martina Azzolini, Marco Angelucci, Roberto Cimino, Rosanna Larciprete, Nicola M Pugno, Simone Taioli, Maurizio Dapor, Journal of Physics: Condensed Matter 31, 055901 (2019)
- Theoretical estimates of Stellar e–Captures. I. The half-life of 7Be in evolved stars, Stefano Simonucci, Simone Taioli, Sara Palmerini, Maurizio Busso, The Astrophysical Journal 764 (2), 118 (2013)
- Electron spectroscopies and inelastic processes in nanoclusters and solids: theory and experiment, Simone Taioli, Stefano Simonucci, Lucia Calliari, Maurizio Dapor, Physics Reports 493 (5), 237-319 (2010)

Dr. **Jonathan Dubois**
Quantum Coherent Device Physics Group Leader, Lawrence Livermore National Lab, Livermore Ca 94550

Recent and ongoing projects:

- 2015- (PI) LLNL Strategic initiative: "Enhanced coherence for quantum sensing and simulation": Developed capability to design fabrication and characterize superconducting quantum coherent devices with applications in quantum sensing, quantum simulation and quantum computation
- 2016- (PI) DOE/NNSA Advanced Simulation and Computing: "Beyond Moore's law computing": Developing algorithms and quantum hardware architectures for quantum simulation.
- 2017- (PI) DOE Advanced Scientific and Computing Research: "Quantum testbed pathfinder program": Evaluation of hardware requirements for realization of quantum simulation algorithms, development of and demonstration of optimized architecture for many-body quantum simulation.

Publications related to the project:

1. Overcoming the fermion sign problem in homogeneous systems, JL DuBois, EW Brown, BJ Alder, Advances in the Computational Sciences: Proceedings of the Symposium in Honor of Dr Berni Alder's 90th Birthday. World Scientific, (2017).
2. Number-squeezed and fragmented states of strongly interacting bosons in a double well, JC Corbo, JL DuBois, KB Whaley, PRA 96 (5), 053627 (2017)
3. DOE workshop on Materials Frontiers to Empower Quantum Computing, Report, Jun (2015)

Dr. **Kyle Wendt**
Lawrence Fellow, Lawrence Livermore National Lab, Livermore CA 94550
Recent and ongoing projects:

- 2017- (PI) LLNL Lawrence Fellowship Exploratory Research LDRD: "Laying the Foundation for a Predictive Theory of Electroweak Nuclear Phenomena"
- 2018- (co-PI) LLNL Exploratory Research LDRD: "Beta Decay at the Limits of Nuclear Stability"
- 2018- Nuclear Dynamics on a Quantum Chip

Publications related to the project:

1. Discrepancy between experimental and theoretical β-decay rates resolved from first principles, P. Gysbers, G. Hagen, J. D. Holt, G. R. Jansen, T. D. Morris, P. Navrátil, T. Papenbrock, S. Quaglioni, A. Schwenk, S. R. Stroberg, K. A. Wendt Nature Physics (2019)
2. Coupled-cluster calculations of nucleonic matter, G. Hagen, T. Papenbrock, A. Ekström, K. A. Wendt, G. Baardsen, S. Gandolfi, M. Hjorth-Jensen, and C. J. Horowitz, Phys. Rev. C 89, 014319 (2014)
3. Charge, neutron, and weak size of the atomic nucleus, G. Hagen, A. Ekström, C. Forssén, G. R. Jansen, W. Nazarewicz, T. Papenbrock, K. A. Wendt, S. Bacca, N. Barnea, B. Carlsson, C. Drischler, K. Hebeler, M. Hjorth-Jensen, M. Miorelli, G. Orlandini, A. Schwenk, and J. Simonis, Nature Physics 12, 186-190 (2016)

8. The project is relevant for the following Q@TN work-package(s):

1. WP4: Quantum simulations, area of action: QS for nuclear and sub-nuclear physics
2. WP3: Quantum computing, area of action: Computer architecture
3. WP1: Fundamental quantum science, area of action: Quantum Many-Body Physics

9. Description of the project

Control-centric quantum computing is based on the idea that arbitrary "gates" acting on a qubit can be realized by applying some external time dependent control signal (that we can consider as the "low-level software") to a predetermined quantum system (the "hardware"), in such a way that the resulting propagation reproduces the effect of a an Hamiltonian of choice.
This scheme naturally includes in itself that of universal quantum machines (the low-level software might simply encode the effect of standard quantum gates), and it extends it to the possibility of using arbitrary unitary transformations, which in the present NISQ era represents a more efficient way of reaching some practical application of quantum computing. The quantum testbed that has been built at Lawrence Livermore National Laboratory, based on multilevel transmons realized in a cryogenic GHz cavity coupled to an external highly tunable pulse generator, envisions to become a first concrete realization of this quantum computation scheme.

More in detail, given a quantum machine based on circuit QED and defined by a Hamiltonian:

$$H_0 \approx \sum_i^N \omega_i a_i^\dagger a_i - \chi_{ii} a_i^\dagger a_i^\dagger a_i a_i - \sum_{j \neq i}^N \chi_{ij} a_i^\dagger a_i a_j^\dagger a_j$$

where the parameters ω, and χ are intrinsic properties of the circuit, we want to generate a unitary transformation U_{target} having the effect of time propagating the system with a Hamiltonian H of our choice. Universal quantum computers[1] define a specific subset of these operations, but we want to consider a completely general case. To this end, we couple our system to an external pulse generator (which we might assume to be described by an Hamiltonian H_c), with a time dependent coupling[2]. The resulting propagator is given by:

$$U_{target} \approx \int_0^T e^{it(\hat{H}_0 + f(t,\alpha)\hat{H}_c)} dt$$

where the α are parameters of the Hamiltonian we want to simulate. This integral equation needs to be solved for the function $f(t,\alpha)$, which has in turn to be fed to the pulse generator in order to implement the desired gate. There are several algorithms available to perform this operation. In the machine-level simulations of the LLNL testbed and for the preliminary measurements the GRAPE (Gradient Ascent Pulse Engineering) package, publicly available in Python, was used. The computing time for solving this integral problem scales exponentially with the dimensionality of the Hilbert space on which the Hamiltonian is defined. While we recently showed that this control-centric approach can be formulated in such a way to beat the exponential scaling of the computational cost arising, for instance, from a non-trivial spin structure of the Hamiltonian such that needed to describe many-nucleon systems, the curse of exponential scaling seems to appear again in the determination of the controlling function itself.

In the case we are interested in simulating time-dependent processes (e.g. nuclear reactions, chemical reactions, ab-initio lattice dynamics in solids, etc.), this might seem a serious application killer. However, let us consider for simplification the case of *ab-initio* lattice dynamics. Let us suppose that the control-centric procedure allows to solve for the propagation of the electronic structure of a given N-ion configuration in one single gate application, and that forces can be computed to move the ions in turn. For the next step we need to recompute the driving pulse for propagating the electrons, and the cost of the simulation would still be exponential in N. However, as widely exploited in the literature (see e.g. Car-Parrinello methods), the electron Hamiltonian can be considered as continuously varying as a function of the ion positions, and his allows for reducing computational costs by exploiting these continuity features. A similar situation can be found if we think of studying the scattering of two nuclei, where one could exploit techniques factorizing the motion of the projectile/target/fragment center of mass, leading to similar considerations.

These examples illustrate the general aim of the proposal. We intend to study general schemes to accelerate the determination of a control pulse in a control-centric quantum computing scheme to help

avoiding the exponential increase in computing cost (on classical machines) as a function of the increase of the size of the system.
This problem has been attacked in the past by several groups[3].

On a more concrete level, we want to find some set of parameters α that encode a unitary matrix $U(\alpha)$ which approximates the time evolution operator U of a targeted Hamiltonian H. The unitary matrix in principle (U) has more degrees of freedom than α, and our objective functions that describes how well our $U(\alpha)$ describes U is relatively expensive to compute. Machine Learning (ML) techniques are well suited to accomplish this goal.

The first goal will be to apply supervised learning as a surrogate to speed up the process of finding the optimal α for a given U. The idea is to build a smooth map from specific features of H (e.g. positions of particles or a coupling constant) to regions of the control parameters α. This approach will be certainly applicable for smaller problems, such as the dynamics of two to four nucleons. As a first test, this method will be applied to the scattering of two neutrons where we only have two features to map, the length and azimuthal angle of the interparticle separation.

As the problem size grows, the number of features we need to map will grow rapidly and supervised learning will become infeasible. Instead, one can look at how to cluster Hamiltonians together and then study how the clusters each individually map between the physical feature and control parameter spaces. Another alternative is to apply unsupervised learning tools such as autoencoders and generative models as tools to map the exponentially large feature space to a smaller and more manageable synthetic feature space.

An obvious question here concerns the level of detail that is required in the determination of the pulse in order to obtain the desired propagator. Besides some technical limits related to the resolution of the pulse generator itself, any fitting procedure might produce deviations that in turn generate errors in the propagation. It will be necessary to develop a way to understand and quantify in a precise manner such errors, so that it will be possible to have better tuning of the computational resources to be used in a practical application. Once these aspects have been carefully studied, the precision requirements can be easily included in the definition of the cost function in a ML scheme.

This project is well suited for a Ph.D. student, who would have a unique opportunity to develop a working experience in two of the most exciting fields in contemporary computational methods: quantum computing and machine learning. In fact, the student's work would not be limited to the development and implementation of ML techniques for control theory in an abstract context, but it would also involve following and participating in forms that will be defined in the practical implementation of her/his achievements on the LLNL quantum testbed, with the possibility of visiting the site. At the local level the student would be inserted in the context of the Physics Department, and of the research group LISC at ECT*, besides become associated to INFN in the Trento Institute for Fundamental Physics and Applications (TIFPA) center.

The main deliverables and milestones in the three Ph.D. years would be the following:

Year one/first half of year two: Theoretical assessment of the sensitivity of the unitary operations generated on the LLNL quantum testbed on the accuracy of the generated pulse, and analysis of the error propagation. Development of an appropriate cost function for appropriately constraining the pulse within the minimum standard of accuracy by supervised ML methods. Tests at device simulation level on the two interacting neutron problem, and consistency checks. First tests on the quantum testbed.
Second half of year two/beginning of year three: Extension of the devised scheme to more complex problems, and consequently on wider parameter space. In particular we aim to target the problem of reactions between light nuclei and dynamics of simple molecules, in order to demonstrate the viability of

the general scheme and proving scaling properties inclusive of the classical computing time necessary to solve for the control pulse.
Year three, second half: Study of possible unsupervised ML schemes for the case of a large number of parameters. The student at this time will be mostly focused in the writing of the thesis.

References:
[1] S. Lloyd*, "Universal Quantum Simulators",* Science 273, 1073-1078 (1996)
[2] For a review see e.g. S. Schirmer*, "Hamiltonian Engineering for Quantum Systems",* in: Allgüwer F. et al. (eds) *Lagrangian and Hamiltonian Methods for Nonlinear Control 2006. Lecture Notes in Control and Information Sciences*, vol 366. Springer, Berlin, Heidelberg
[3] See e.g. M. Bukov, A. G. R. Day, D. Sels, P. Weinberg, A. Polkovnikov, and P. Mehta "Reinforcement Learning in Different Phases of Quantum Control", Phys. Rev. X 8, 031086 (2018)

10. Interdisciplinary aspects
The project team will involve researcher at FBK/ECT * (Dr. Simone Taioli) and at the Physics Department of the University of Trento (prof. Francesco Pederiva), in strict cooperation with staff at Lawrence Livermore National Laboratory (Dr. Jonathan Dubois and Dr. Kyle Wendt). The interdisciplinarity of the project is evident. The aim of the research is essentially a technological development allowing to overcome some difficulties intrinsic in the control-centric quantum computing scheme, and the results will be directly applied to the functioning of the hardware existing at LLNL.
The competences that need to be involved here are multiple. A detailed knowledge of the technicalities related to the experiment are necessary to understand at which level the cost functions that define the ML procedure need to be tuned in order to give results usable at hardware level. Together with that it is necessary to have a good understanding of the theory underlying the control process. This competence is pertinence of the LLNL partners (in particular Dr. Dubois). Another obvious aspect of this project is the use and development of mathematical and practical aspect of machine learning techniques. In the team this aspect will be supervised by Dr. Simone Taioli at ECT*. Finally, we need competence in both the understanding of general aspects of time-dependent many body problems (nuclear reactions and dynamic evolution of solids) and all the software related problems that allow for treating a realistic many-body problem. All the team members are experts in different aspects of this field.
If fully successful the project has a substantial potential for impacting research in different disciplines, not only in the sense of different branch of physics, but also chemistry, materials science, and also quantum information theory in a broad sense.

11. Relevance of the project for quantum science and technology
As previously mentioned in the text, this project has a potential to significantly impact the development of quantum computing in the next few years. Given the state of the art of quantum hardware, a practical implementation of a universal quantum computer is still several years away. The control-centric scheme that we have recently proposed has conceptually the power of at least bridging this time gap. However, the unfavourable scaling related to the need of generating the control pulses might prevent a sufficiently rapid development. A positive outcome of this project would help to go over this shortcoming, substantially improving the scaling with the number of qubits, and would open the door to a widespread application. The potential impact is very strong, not only in the field of nuclear dynamics (impacting all studies related to dense matter phenomenology), but also for as concerns the study of ab-initio dynamics in molecular systems and solids, with obvious consequences on the capability of engineering new materials for technological applications.
The interest in quantum computing in all aspects is testified by the investments that the US DoE recently made, specifically in the area of nuclear physics and lattice QCD. The first papers/preprints on the subject have already been published, and it would be important to have a chance not to be cut out of this growing trend, which will probably represent the future of nuclear physics in the following years.

12. Possible referees

Prof. Martin Savage
Institute for Nuclear Theory
University of Washington
Seattle, WA (USA)
Email: mjs5@uw.edu

Dr. Pavel Lougovski
Computational Sciences and Engineering Division
Oak Ridge National Laboratory
Oak Ridge, TN (USA)
Email: lougovskip@ornl.gov

Prof. Alan Aspuru-Guzik
Dpt. of Chemistry and Dpt. of Computer Science
University of Toronto
Toronto, ON (Canada)
Email: alan@aspuru.com