

# A new generation of HPC developers using quantum Monte Carlo (QMC) methods is growing

## Outcomes of the first TREX e-School on Quantum Monte Carlo with TurboRVB

*Quantum Monte Carlo (QMC) methods have never been so appealing according to the engagement rate of the first edition of the TREX e-School on Quantum Monte Carlo. Jointly organised by TREX, the Centre of Excellence in Exascale Computing for quantum chemistry and materials science, together with the Psi-k network and the International School for Advanced Studies (SISSA), from 12 to 16 July 2021 the virtual summer school hosted 66 students and trained 24 selected applicants in using TurboRVB as the main code for QMC applications and tutorials.*

### August 2021

Quantum Monte Carlo (QMC) methods belong to one of the most accurate families of numerical approaches for materials and electronic structure calculations. Moreover, the steady increase of computer power in HPC machines is very much suitable for the development and usage of stochastic ab initio methods, which - beside the high precision - are highly parallelizable and enjoy a favorable scaling with the system size. To build a large user community, it is of paramount importance to disseminate the knowledge, information, and practice of this kind of methods, particularly among students and young researchers.

**With this target in mind, from 12 to 16 July TREX, the Centre of Excellence in Exascale Computing for quantum chemistry, organised the first e-School on Quantum Monte Carlo, training students to use TurboRVB as the main code for QMC applications and tutorials, a unique opportunity to provide a comprehensive introduction to QMC methods without any prerequisite. The e-School was sponsored by the TREX project, the [Psi-k network](#) and SISSA, the [International School for Advanced Studies](#) located in Trieste, Italy.**

89 valid applications were received from Postdoc students, Master Students, researchers, and HPC experts for the online summer school, of which 66 (from 33 countries and 4 continents) were admitted to the public plenary lectures and 24 were selected to follow the hands-on tutorials in the afternoons. More than 50 students connected each day to follow the lectures, an excellent engagement rate.

*“The TREX e-school was a great opportunity to learn the theories underlying quantum Monte Carlo calculations and start using TurboRVB in well-organized hands-on sessions” Says Sarah (Fatemeh) Keshavarz, computational chemist with PhD degree in the field of Physical Chemistry from Shiraz University (Iran). “The e-school seemed like an intense course. But the explanations were clear and well-balanced for both researchers with limited knowledge of the underlying theories and those knowledgeable in the field.”*



### About Turbo RVB

[TurboRVB](#) is a computational package for ab initio Quantum Monte Carlo (QMC) simulations of both molecular and bulk electronic systems. The code implements two types of well established QMC algorithms: Variational Monte Carlo (VMC), and Diffusion Monte Carlo in its robust and efficient lattice regularized variant.

During the 5 morning plenary sessions, open to all participants, Michele Casula, CNRS, Sandro Sorella and Kosuke Nakano, SISSA and five additional lecturers provided undergraduate students with a basic but detailed overview of the theoretical foundations of QMC computer simulations and of the domains of application. The lectures served as an introduction for the Hands-on session in the afternoon, open to 24 selected students providing the basics for writing and running in practice simulations using TurboRVB as in-house quantum Monte Carlo code.

*"The quantum Monte Carlo TurboRVB e-school has been very fruitful for all participants and teachers" says [Michele Casula](#), member of the Programme Committee and one of the lecturers at the school. "As a lecturer, I am happy that this event has been followed on-line by people all over the world, with a great participation and a constant number of attendees during the whole week. It was a good mix of general introduction to quantum Monte Carlo, explanations of the original wave functions and algorithms coded in the TurboRVB package, and useful hands-on sessions to start working with TurboRVB. I hope that this will become a regular event, organized with an annual or bi-annual schedule, to build a stronger community around quantum Monte Carlo and TurboRVB."*

All material from the plenary sessions is [available online](#) while a training area is being populated. In November 2021, TREX is organising a [Hackathon](#) on how to use build systems (such as [CMake](#) and [GNU Autotools](#)) to improve the portability of applications. Stay tuned on <https://trex-coe.eu/>

### About TREX

TREX has been awarded the Center of Excellence in Exascale Computing for the community of quantum chemistry. TREX federates European scientists, High Performance Computing stakeholders, and SMEs to develop and apply high-performance software solutions for quantum mechanical simulations at the exascale. The final goal of the project is to develop a set of flagship Quantum Monte Carlo codes, able to exploit the capabilities of the recent exascale computers at its highest.

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