QSE – A Python package for lattice-based simulations and calculations

James Nelson
Sherry Blair

Irish Centre for High-End Computing (ICHEC), Dublin, Ireland

james.nelson@ichec.ie
sherry.blair@ichec.ie

QSE [1,2] (Quantum Simulation Environment) is an open-source python package developed at ICHEC by the Quantum-HPC team as part of the HPCQS project [3]. It is adapted from the Atomic Simulation Environment (ASE) package for setting up, steering, and analysing atomistic simulation, keeping the flexibility and ease of use of ASE.

The goal of QSE is to support a wide range of quantum simulations through a variety of backends in a vendor-agnostic way. QSE can interact with several quantum computing SDKs such as Pulser and myQLM (particularly well-suited for analog quantum computation), Qiskit (for digital quantum computing), and Qutip (for software-based quantum emulation).

The central object in QSE is the Qbits class which contains information about the geometry of the system. From this class, one can run a number of calculations. For example, simulations of neutral atom systems where the interaction Hamiltonian is described by a power law based on the distance between the qubits [4], or spin models with nearest neighbour interactions based on the geometry.

QSE also supports several post processing functions which allow one to calculate various expectation values and correlation functions, and to be able to visualize such quantities.

Figures

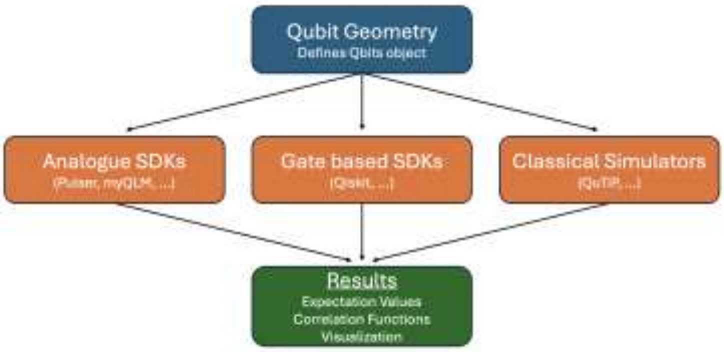

Figure 1: The geometry of the qubits defines the Qbits object, which can be then passed to various backends. In addition QSE supports various tools to interpret the results.

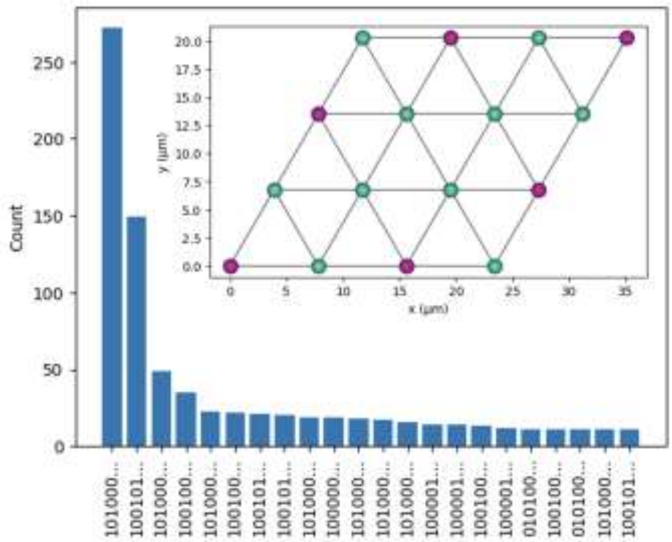

Figure 2: An illustration of an analogue quantum computing simulation. The bar chart shows the distribution of measurements, and the insert shows the corresponding lattice for the system with the colouring reflecting the Rydberg states 0 (ground) and 1 (excited) of the most frequently measured state.

References

[1] https://github.com/ICHEC/qse/
[2] https://ichec.github.io/qse/
[3] https://hpcqs.eu
[4] Browaeys, A. & Lahaye, T. *Nature Physics* 16, 132–142 (2020).