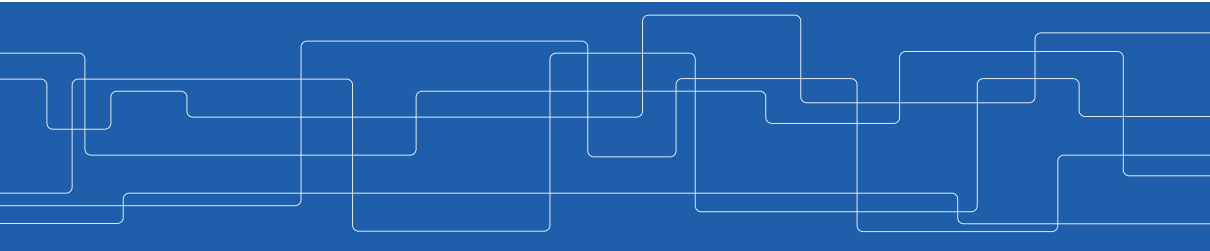
CERN openlab

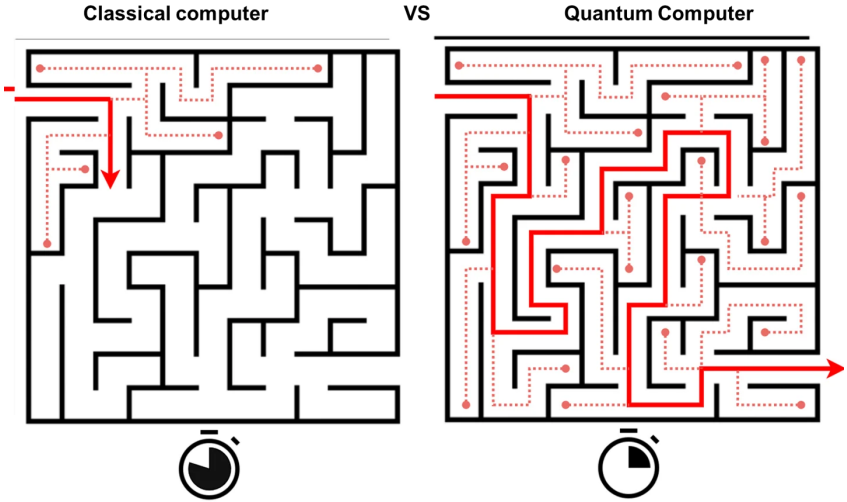
QUANTUM TECHNOLOGY INITIATIVE

Speeding-up simulations of quantum algorithms for material science

Gehad Ahmed
Supervisors: Carla Rieger, Michele Grossi



Quantum Computing vs Classical Computing

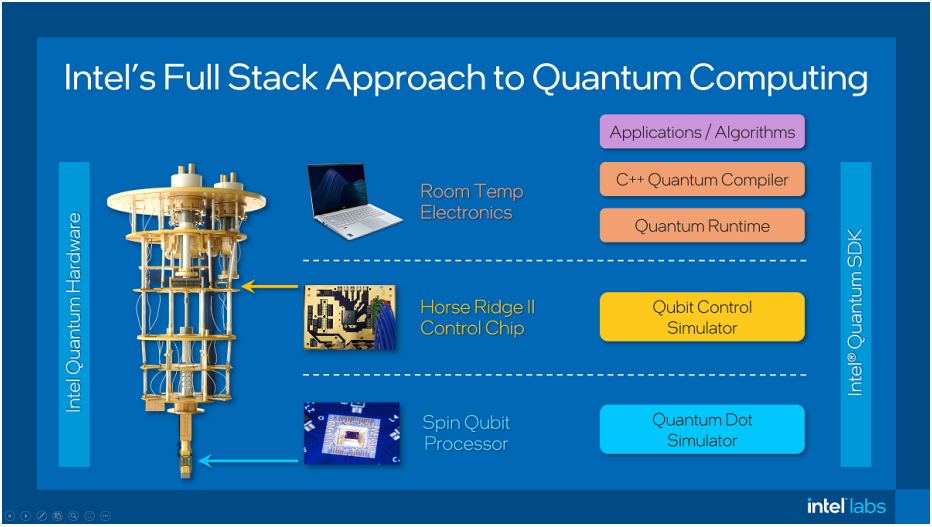


www.swidch.com/resources/blogs/quantum-proofing-our-secrets-safeguarding-communication-in-the-age-of-quantum-computers

Quantum Simulations on Classical Computers

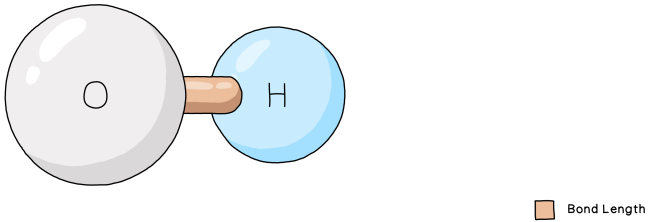
- Simulating an ideal quantum computer, with no noise/errors.
- Benchmarking/simulating a real quantum computer, matching its noise & error rate.
- Simulating proposed enhancements to an existing quantum computer.
- Debugging a quantum circuit.

Intel Quantum Simulator SDK



https://www.hpcwire.com/wp-content/uploads/2022/09/Intel_Quantum_Computing-675x380.png

OH- Molecule

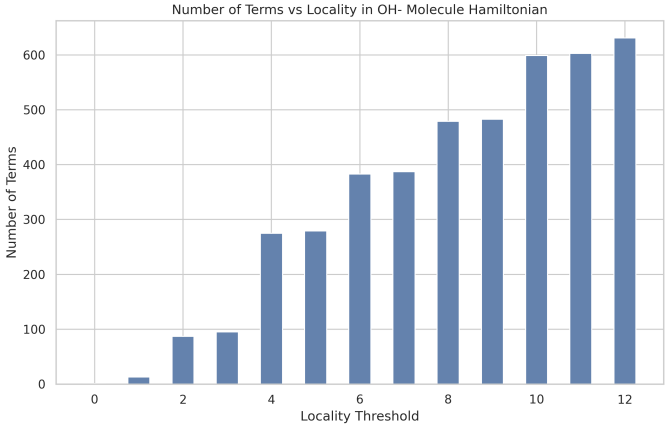


- Its dynamics is represented by a Hamiltonian (operator corresponding to the total energy of the system) over 12 qubits.

https://pennylane.ai/datasets/qchem/oh-anion

Locality in OH- Molecule

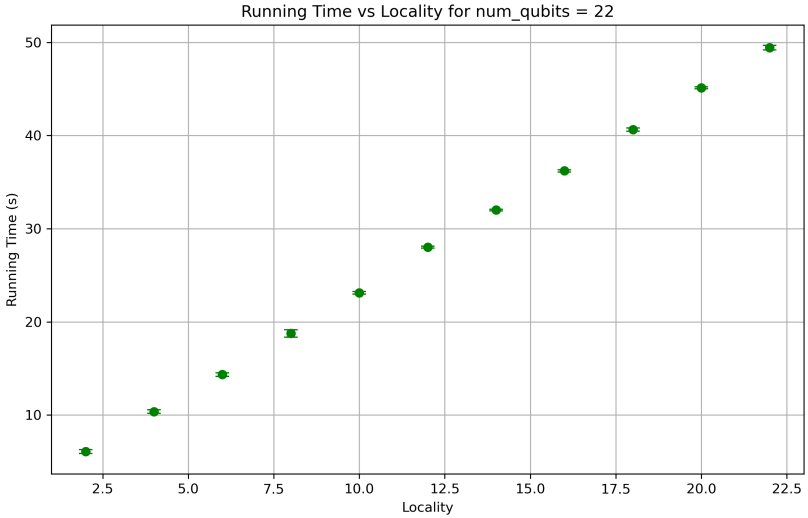
- The locality over a term is the number of (non-trivial) rotations acting the qubits.
- The locality of the Hamiltonian is the maximum locality over all terms.



Integration with Intel Quantum SDK

- Hamiltonian Parsing.
- Translating the Hamiltonian into a gate-based quantum circuit.
- C++ Code Generation.
- Compilation over Intel Quantum SDK.

Random Hamiltonians with 22 qubits and 50 terms



Further work

- Run the circuits for the OH- molecule after the patch update in Intel SDK for the compiler.
- Run analysis over the Intel SDK with a novel multi-qubit rotation configuration.
- Benchmark the multi-qubit rotation against the single and double-qubit rotation configuration in terms of compilation and running times.

Thank You!

Your questions are welcome!

Gehad Ahmed
gehad.ahmed@cern.ch
gehadsalemfekry@aucegypt.edu