High Performance Simulations of Quantum Computing
Why are they important?

Simulations are crucial for:

- Development of quantum computers
- Verification of algorithms and hardware
- Defining the *quantum advantage*
- Understanding quantum systems
- Noise modelling

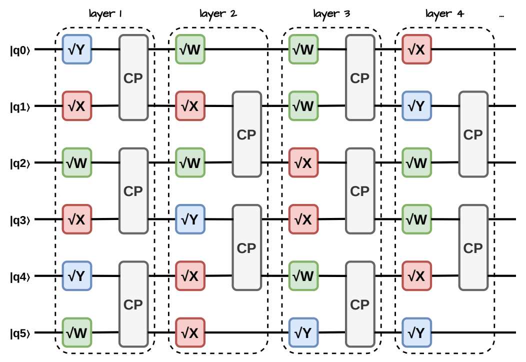
Coming soon (maybe) – *quantum processing units (QPUs)* as accelerators in HPC systems.

My PhD project focuses on:

- Existing simulators experiments
- Developing a new simulation framework
- Testing quantum models with it
- Pushing the limits of simulations

Benchmarking *quantum advantage* with:

- **Quantum Fourier transform (QFT)** [1]
  Common subroutine in quantum algorithms
- **Random circuit sampling (RCS/RAND)**
  Simplified version of Google's circuit [2]:



What approaches are there?

I. Statevector evolution:

- **The Schrödinger's approach:**
  Needs $\mathcal{O}(2^n)$ memory for n qubits
- **The Feynman path approach:**
  Needs $\mathcal{O}(4^d)$ time for d gates
- **The combined approach:**
  Splits the state into 2 parts; uses the Schrödinger's method within each, and the Feynman's method for interconnections

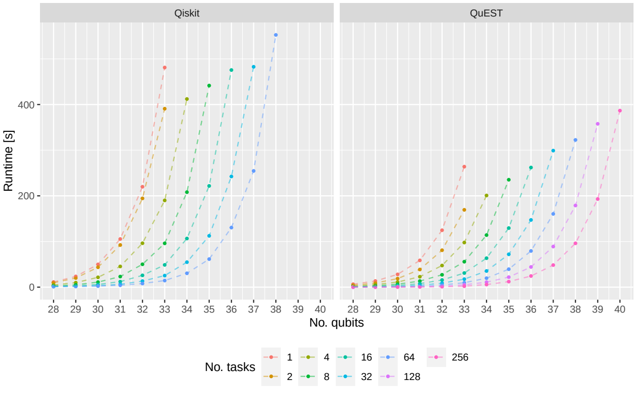
ARCHER2 (1 PB of RAM) can store max 44 qubits (maybe 45) with the Schrödinger's method.

To simulate Google's 53 qubits, the combined approach needed – would take 10,000 years [2].

Qiskit [3] and QuEST [4] software.

Both distributed with MPI:
QuEST uses huge messages; Qiskit swaps the state with *cache blocking* [5].

QuEST up to 2 times faster for QFT simulation.

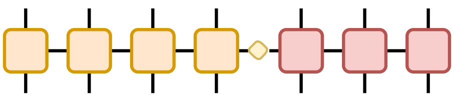


II. Tensor network (TN) contraction:

- Generalisation of the statevector method
- Arbitrary gate application order
- Best with *optimal contraction order*
- *Precomputes* reusable parts (unless too much memory used)
- Can be sped up by approximation

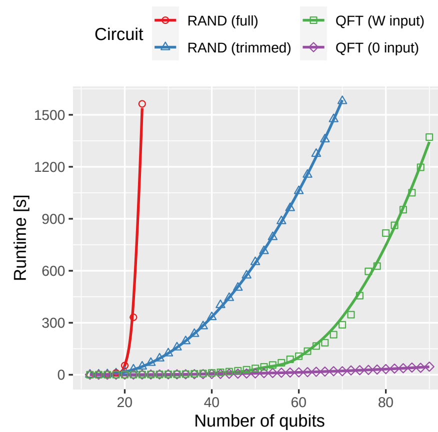
Managed to beat Google's random sampling! [6]

Decompose TNs to **matrix product states (MPSs)** and **matrix product operators (MPOs)** – explicit control of the entanglement. [7]



ITensor software [8] – sequential, but can still show exponential speedup (sometimes).

Truncate the entanglement to insert *decoherence noise*, and reduce runtime.



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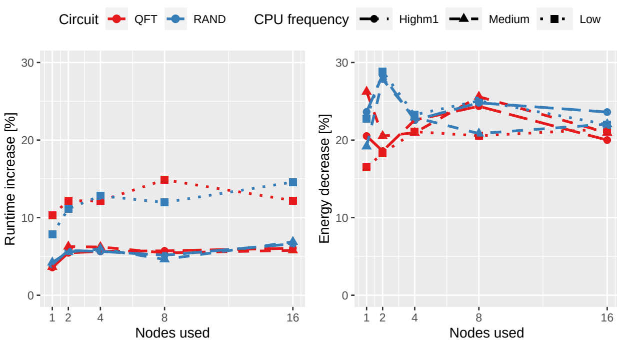
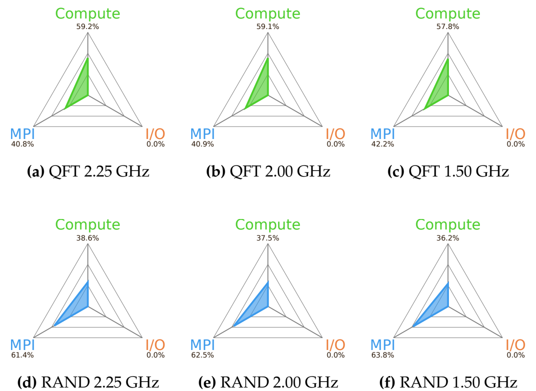
How to execute them efficiently?

CPU downclocking – large energy savings at small runtime penalty.



Works well when the problem is not largely *compute bound* – e.g. statevector simulation.

ARM MAP profiles of QFT and RAND:



(a) QFT 2.25 GHz **(b)** QFT 2.00 GHz **(c)** QFT 1.50 GHz

(d) RAND 2.25 GHz **(e)** RAND 2.00 GHz **(f)** RAND 1.50 GHz

Other options:

- Swap gates to reduce communication
- Decrease TN accuracy

Acknowledgements and References

This work used the ARCHER2 UK National Supercomputing Service (`https://www.archer2.ac.uk`).

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