PH 441
2020

Lecture 1

Nature isn't classical, dammit,
and if you want to make a simulation of nature,
you'd better make it quantum mechanical.

Richard Feynman

Classical computing is what drives smartphones, laptops, Internet servers, mainframes, high performance computers, and even the processors in automobiles.

A quantum bit, more commonly known as a qubit, is a two-state quantum system. It extends and complements the classical computing notion of bit, which can only be 0 or 1. The qubit is the basic information unit in quantum computing.

FANTASY?

What if we could do chemistry inside a computer instead of in a test tube or beaker in the laboratory? What if running a new experiment was as simple as running an app and having it complete in a few seconds?

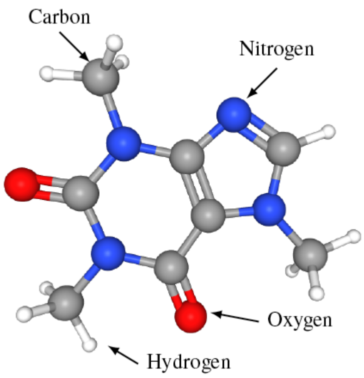
For this to really work, we would want it to happen with full fidelity. The atoms and molecules as modeled in the computer should behave exactly like they do in the test tube. The chemical reactions that happen in the physical world would have precise computational analogs. We would need a fully faithful simulation.

If we could do this at scale, we might be able to compute the molecules we want and need. These might be for new materials for shampoos or even alloys for cars and airplanes. Perhaps we could more efficiently discover medicines that are customized to your exact physiology. Maybe we could get better insight into how proteins fold, thereby understanding their function, and possibly creating custom enzymes to positively change our body chemistry.

How reasonable these fantasies are? (*After all, fantasies are always fantasies! ☺*)

We have massive supercomputers that can run all kinds of simulations. Can we model molecules in the above ways today?
Let's start with $C_8H_{10}N_4O_2$ – 1,3,7-Trimethylxanthine. This is a very fancy name for a molecule which millions of people around the world enjoy every day: caffeine. An 8 ounce cup of coffee contains approximately 95 mg of caffeine, and

this translates to roughly 2.95×10^{20} molecules. A 12-ounce can of a popular cola drink has 32 mg of caffeine, the diet version has 42 mg, and energy drinks often have about 77 mg. (Please note that that there are between 10^{49} and 10^{50} atoms in our planet alone.)



Can we model caffeine exactly in a computer? We don't have to model the huge number of caffeine molecules in a cup of coffee, but can we fully represent a single molecule at a single instant?

Caffeine is a small molecule and contains protons, neutrons, and electrons. In particular, if we just look at the energy configuration that determines the structure of the molecule and the bonds that hold it all together, the amount of information to describe this is staggering. In particular, the number of bits, the 0s and 1s, needed is approximately 10^{48}. This is comparable to 1% to 10% of the number of atoms on the Earth!

This is just one molecule! Yet somehow nature manages to deal quite effectively with all this information. It handles the single caffeine molecule, to all those in your coffee, tea, or soft drink, to every other molecule that makes up you and the world around you. How does it do this?

We don't know!

In the traditional sense, we have no hope of providing storage to hold this much of information. Our dream of exact representation appears to be dashed. This is what Richard Feynman meant!

However, 160 qubits (quantum bits) could hold $2^{160} \approx 1.46\times10^{48}$ bits while the qubits were involved in computation. To be clear, I'm not saying how we would get all the data into those qubits and I'm also not saying how many more we would need to do something interesting with the information. It does give us hope, however.

In the classical case, we will never fully represent the caffeine molecule. In the future, with enough very high quality qubits in a powerful enough quantum computing system, we may be able to perform chemistry in a computer.

Why Quantum Computing is different?

- If you flip a quantum coin and then **don't look at it**, flipping it again will yield the heads or tails with which you started. If you do look, you get classical randomness.

Your phone or laptop uses bytes as the individual units of memory or storage. That's where we get phrases like "megabyte," which means one million bytes of information. A byte is further broken down into eight bits. Each bit can be 0 or 1. Doing the math, each byte can represent $2^8 = 256$ different numbers composed of eight 0s or 1s, but it can only hold one value at a time.

- Eight qubits can represent all 256 values at the same time.

- This is through superposition, but also through *entanglement*, the way we can tightly tie together the behavior of two or more qubits. This is what gives us the (literally) exponential growth in the amount of working memory that we saw with a quantum representation of caffeine.

Summary:

- The lone 1s and 0s of classical computing bits are extended and complemented by the infinite states of qubits, also known as quantum bits.
- The properties of superposition and entanglement give us access to many dimensions of working memory that are unavailable to classical computers.
- Industry use cases for quantum computing are nascent but the areas where experts believe it will be applicable sooner are chemistry, materials science, and financial services. AI is another area where quantum may boost performance for some kinds of calculations.