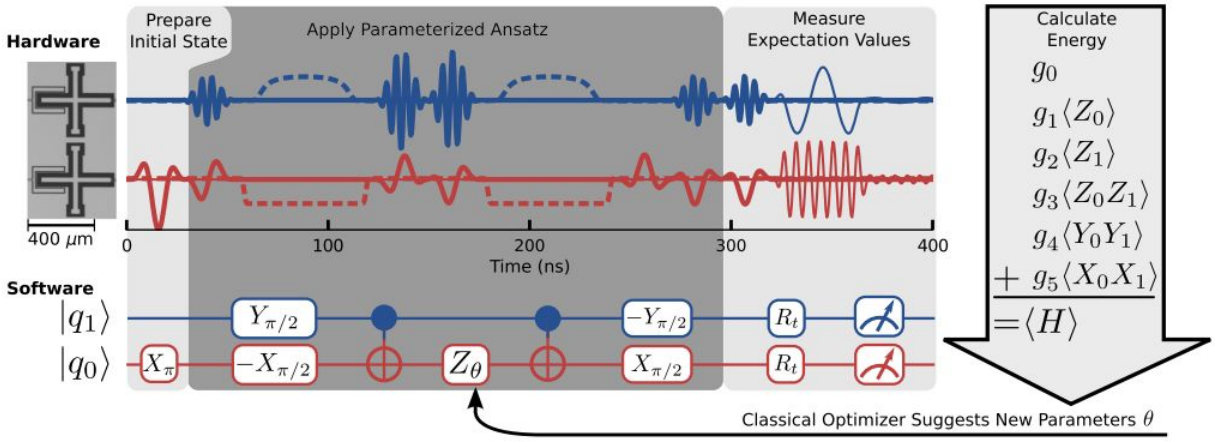
First completely scalable quantum simulation of a molecule

July 20 2016, by Bob Yirka

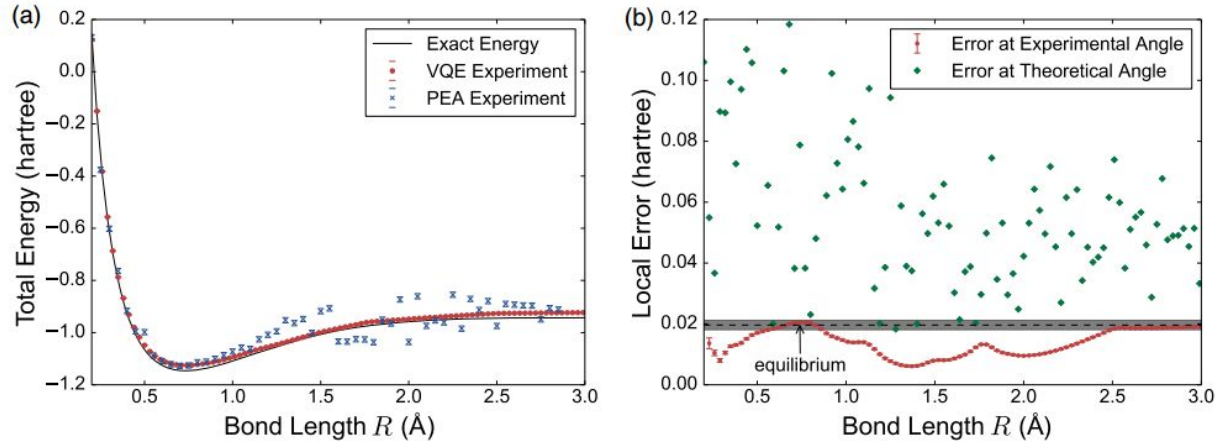


Hardware and software schematic of the variational quantum eigensolver. Credit: *Physical Review X* (2016). DOI: 10.1103/PhysRevX.6.031007

(Phys.org)—A team of researchers made up of representatives from Google, Lawrence Berkeley National Labs, Tufts University, UC Santa Barbara, University College London and Harvard University reports that they have successfully created a scalable quantum simulation of a molecule for the first time ever. In a paper uploaded to the open access journal *Physical Review X*, the team describes the variational quantum eigensolver (VQE) approach they used to create and solve one of the first real-world quantum computer applications.

As research continues with the development of a true quantum computer, some in the field have turned their attention to selecting certain types of problems that such computers could solve, as opposed to what are now being called classical computers. One such problem is solving the molecular electronic structure problem, which as Google Quantum Software Engineer Ryan Babbush notes in a blog post involves searching for the lowest electron energy configuration of a given molecule. What this means in practice is using a machine to compute the energies of molecules—doing so for some, such as methane, is relatively easy and can be done very quickly on a classical computer, but others, such as propane, can take days. This makes it an ideal test case for a quantum computer.

To calculate molecular energies on a quantum computer, the researchers used the VQE approach because it translates well as a quantum equivalent of a neural network, i.e., quantum bits could be used to represent molecular wave functions. Once they had built and programmed the system, they tested it by computing the energy of a hydrogen molecule. Their results very closely matched prior results found using classical computers.



Computed H2 energy curve and errors. Credit: *Physical Review X* (2016). DOI: 10.1103/PhysRevX.6.031007

The researchers are aiming to create a quantum computer that is capable not only of computing single molecule energies, but entire chemical systems. As one example, they would like to be able to simulate what happens as bacteria do their work in producing fertilizer—a process they note that currently consumes approximately 2 percent of global energy produced. That would mean developing a universal quantum computer, which, not coincidently, is a goal Google has set for itself.

More information: P. J. J. O'Malley et al. Scalable Quantum Simulation of Molecular Energies, *Physical Review X* (2016). DOI: 10.1103/PhysRevX.6.031007

ABSTRACT
We report the first electronic structure calculation performed on a quantum computer without exponentially costly precompilation. We use a programmable array of superconducting qubits to compute the energy surface of molecular hydrogen using two distinct quantum algorithms. First, we experimentally execute the unitary coupled cluster method using the variational quantum eigensolver. Our efficient implementation predicts the correct dissociation energy to within chemical accuracy of the numerically exact result. Second, we experimentally demonstrate the canonical quantum algorithm for chemistry, which consists of Trotterization and quantum phase estimation. We compare the experimental performance of these approaches to show clear evidence that the variational quantum eigensolver is robust to certain errors. This error tolerance inspires hope that variational quantum simulations of classically intractable molecules may be viable in the near future.