Universities Space Research Association

Perspectives on Quantum Computing for Chemical Engineering

A Joint View from Academia and Industry

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Quantum Computing Applications in Chemical and Biochemical Engineering

American Institute of Chemical Engineering (AIChE)

Technical University of Denmark

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QUANTUM COMPUTING
APPLICATIONS IN CHEMICAL AND BIOCHEMICAL ENGINEERING WORKSHOP

AIChE
The Global Home of Chemical Engineers

DTU Technical University of Denmark

Motivating paper

This presentation is based on our recent invited perspectives paper for the AIChE Journal

PERSPECTIVE | Full Access

Perspectives of quantum computing for chemical engineering

David E. Bernal, Akshay Ajagekar, Stuart M. Harwood, Spencer T. Stober, Dimitar Trenev, Fengqi You

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Carnegie Mellon University

Cornell University

ExxonMobil Research and Engineering

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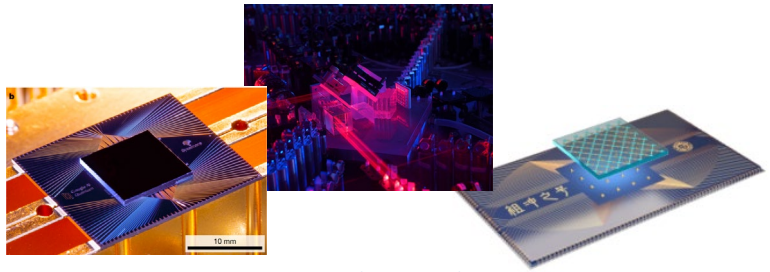
Introduction

- **Practical and functional differences of Quantum Computing (QC) and Classical Computing (CC)**
  - Promise to accelerate certain computational tasks
  - Few available experimental evidence of advantage
- **Significant progress in algorithms driven by research**
  - QC does not extend CC computability, distinction in matter of efficiency
- **Progress in hardware driven by interest from public and private sectors**
- **Progress in software ecosystem driven by growing community**



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Quantum Algorithm Zoo

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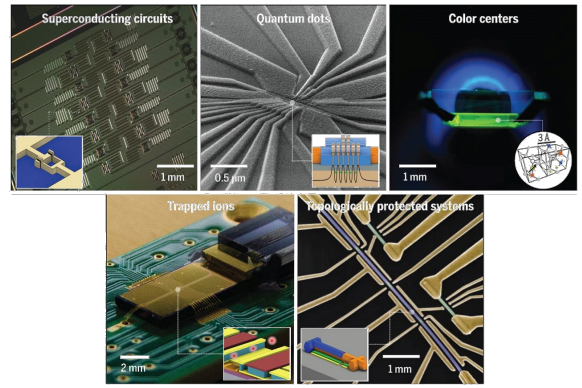


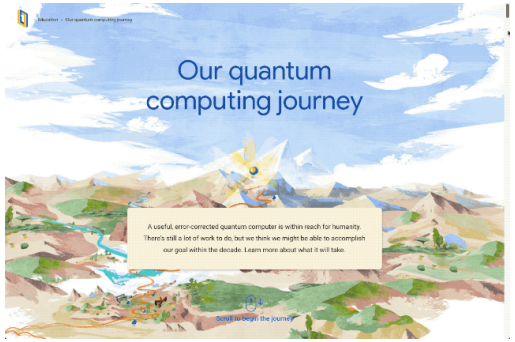
Retrieved from DOI: 10.1126/science.abb2823

qosf

Retrieved from Quantum Open Software Foundation qosf.org/

Introduction

- Progress in 40 years but still not achieving “full promise of QC”
- We are living in the NISQ era
  - Moderate size (~50 qubits) devices
    - Too many for classical simulation
    - Too few for error correction
  - Devices subject to physical noise
    - Distinction of physical and logical qubits
- Fault-tolerance estimated to be reached soon (?)



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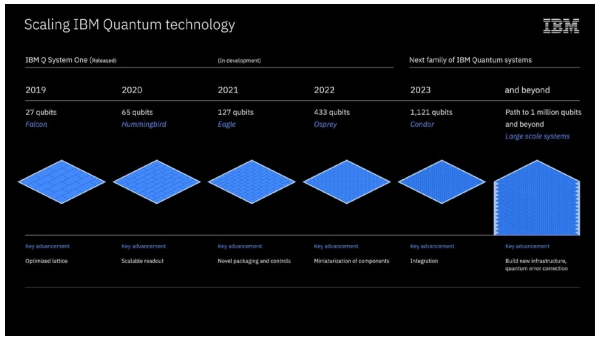
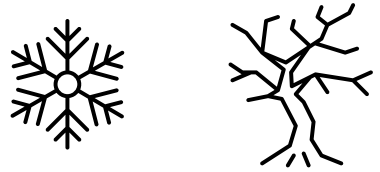


Retrieved from research.ibm.com/blog/ibm-quantum-roadmap

- Advantage experiments highlight the physical possibility of speedups, it is now an engineering challenge
  - Observed for tailored problems, not corresponding to any industrial application yet

Introduction

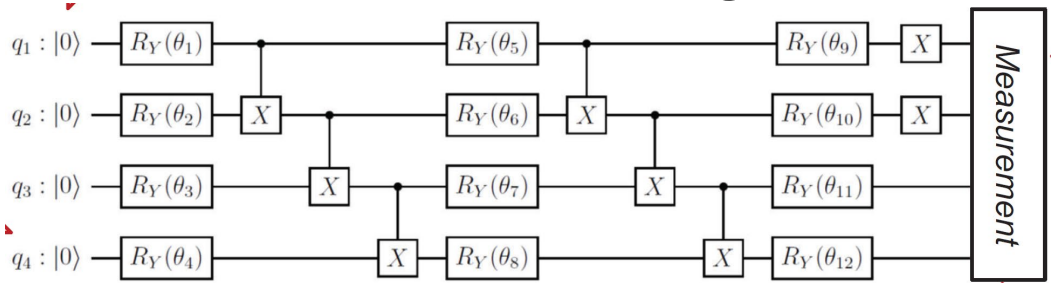
- Chemical industry in privileged position to take early advantage of QC
- Research already in progress in
  - Early-stage experiments to tackle chemical engineering applications
  - Resource estimation for full-scale applications
- Chemical and biomolecular product design may also benefit from QC
  - Chemical property estimation
  - Molecular reaction dynamics
- The growing interest in QC also leads to confusion and hype about its potential and present-day status!!!

- Here we discuss algorithms with potential usage for ChemE and assume that hardware will mature to implement them

Solving problems using Quantum Computing

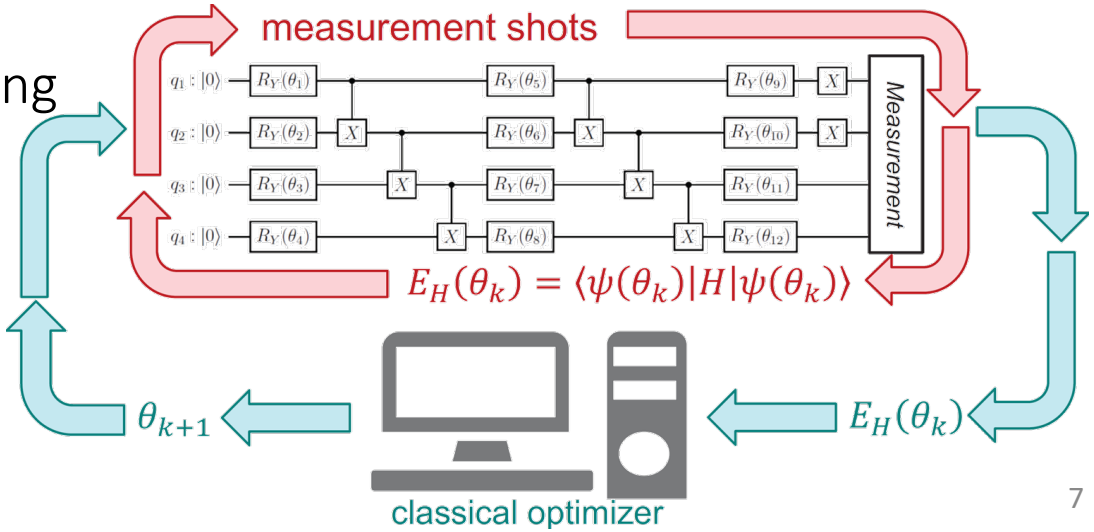
- Definition of Qubits, States, Gates, Circuits, and Algorithms



- QC seems to seamlessly operate on and process information that grows exponentially with number of qubits when running quantum circuits
  - Apparent parallelism!
- Probability amplitudes of qubits can interfere both constructively and destructively
- Main ingredients for theoretical advantage of quantum algorithms
- Examples of such advantages in algorithms for simulation of quantum systems, number factorization, and search and optimization
  - Need not be probabilistic, we use as an example Deutsch-Jozsa algorithm!

Solving problems using current Quantum Computers

- Practical realization of advantage requires implementation of wide and deep circuits
- Current available devices can still be used as shallow circuits that describe probability distributions difficult to represent using CC
- Variational quantum algorithms seem useful in the NISQ era, as outer classical optimization loop to train ansatz can help with devices limitations
- Promising for cases where information is challenging to represent classically
  - Wave functions in computational chemistry
  - Complex distributions to optimize in machine learning



Computational Chemistry and Molecular Simulation

- Many applications in ChemE require kinetic and thermodynamic properties
  - Design and modeling of chemical processes, materials, separations, catalysts, and proteins
- Computational chemistry allows to replace challenging direct measurement and provide molecular-level understanding
- Computational Chemistry believed as first domain where QC may have substantial advantage against CC

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COMPUTATIONAL CHEMISTRY

Chemistry is quantum computing's killer app

Quantum computers could help chemists better understand and develop catalysts, photovoltaics, and more

by Katherine Bourzac

October 30, 2017 | A version of this story appeared in Volume 95, Issue 43

Retrieved from cen.acs.org/articles/95/i43/Chemistry-quantum-computings-killer-app.html

Quantum computing's impact potential and tool used during value creation

Step	1 Design of chemicals[1]	2 Design of products[2]	3 Supply chain	4 Production	5 Marketing
Impact potential	Early killer application	Early killer application	Mature quantum computing	Potential early application	Mature quantum computing
Quantum tool used	• Quantum simulation • Optimization • Quantum AI[3]	• Quantum simulation • Optimization • Quantum AI[3]	• Optimization	• Quantum simulation • Optimization • Quantum AI[3]	• Optimization
Examples of future applications	• Design molecules and solid materials with required properties, reducing lab work • Use computers to define shape of proteins to make better active ingredients	• Discover more effective formulations by modeling how ingredients affect processes or how complex mixtures behave	• Use quantum computing to optimize supply chains and logistics and to reduce costs	• Improve yields and suppress by-product generation through better understanding of reactions and finding new catalysts • Use quantum algorithms to solve complex optimization problems in heat and mass transport	• Use quantum AI[3] to help handle B2B and B2C customer relations

[1]New molecules.
[2]Formulations and complex assemblies.
[3]Artificial intelligence.

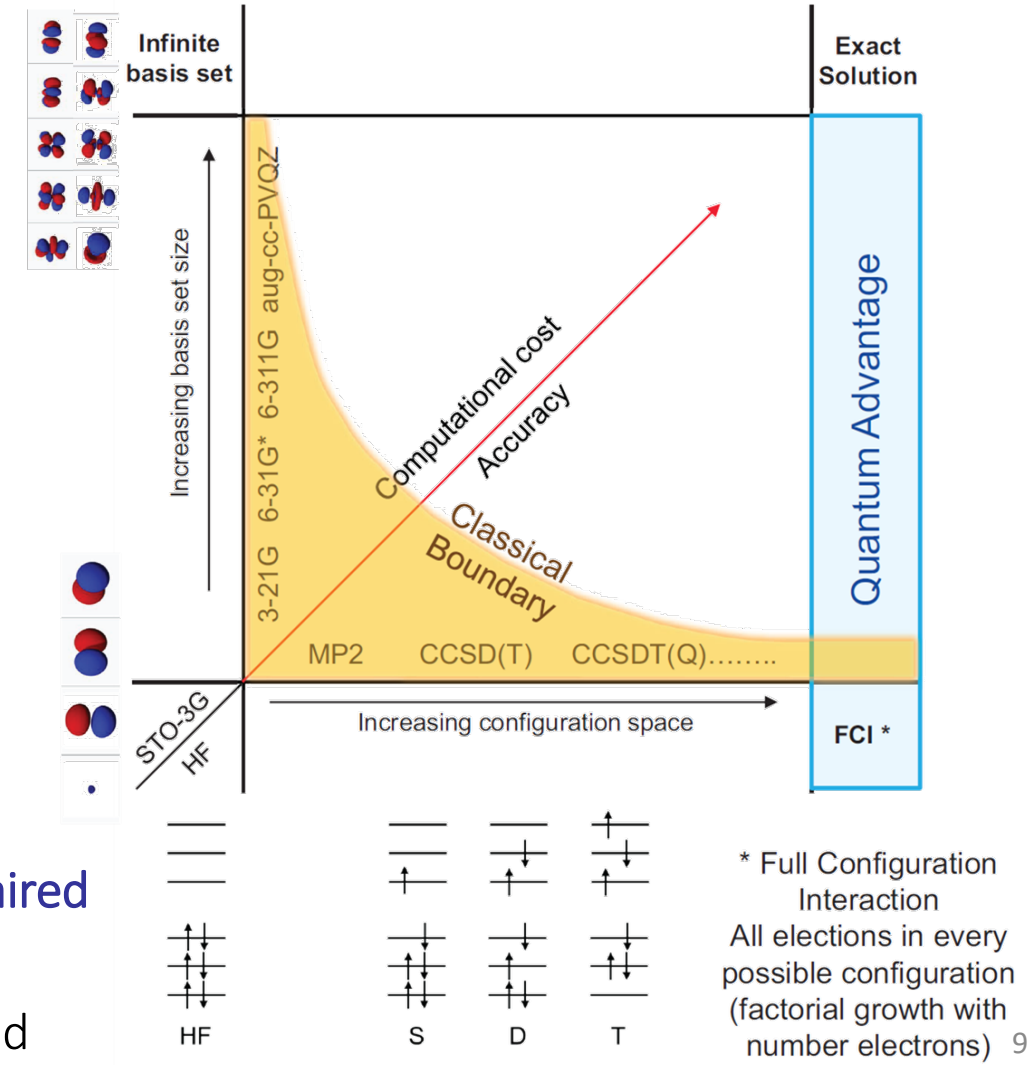
Retrieved from www.mckinsey.com/industries/chemicals/our-insights/the-next-big-thing-quantum-computings-potential-impact-on-chemicals

McKinsey & Company

Computational Chemistry and Molecular Simulation

Typical workflow for estimating kinetic or thermodynamic properties

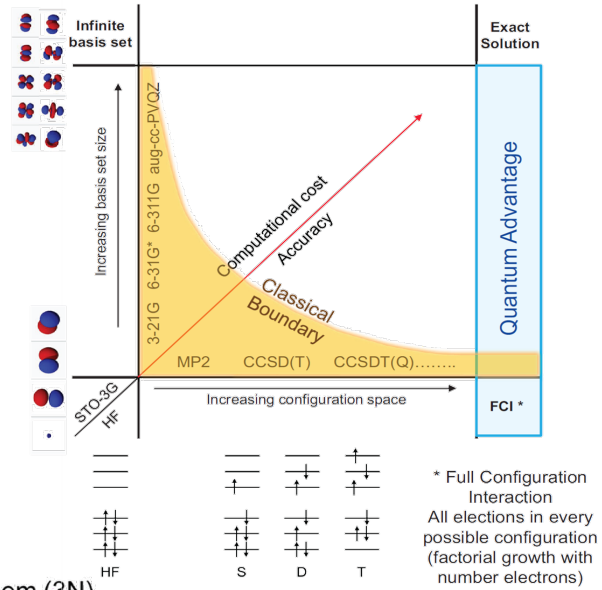
- Choose basis set to represent electrons in system (↑)
  - Usually only valence e^- are modeled and core potential is used for inner e^-
  - Minimally one basis function is used for each valence e^-
    - STO-3G commonly used
    - Usually insufficient
  - Limiting case if infinite basis set
- Choose approximation of Schrödinger eq. (→)
  - Key attribute is degree of electron correlation
    - Hartree-Fock approximation, no excitations and all e^- paired
    - Usually insufficient
  - Limiting case full configurations interactions (FCI) considered

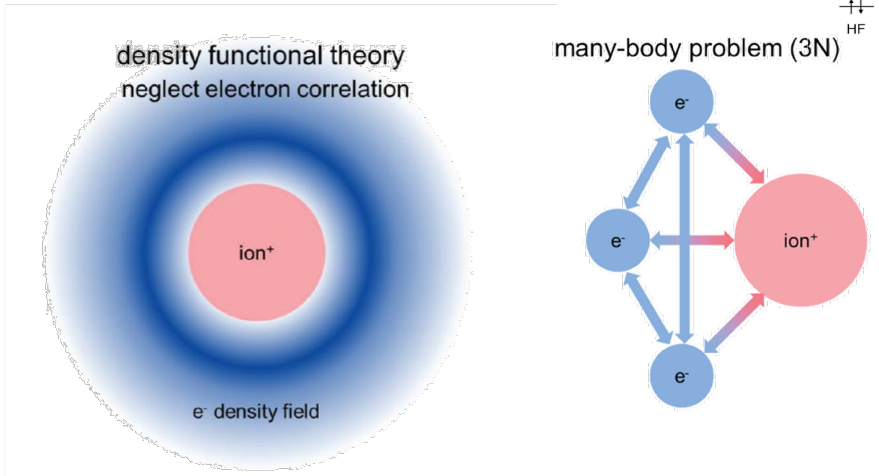


Computational Chemistry and Molecular Simulation

Typical workflow for estimating kinetic or thermodynamic properties

- Exact solutions are limiting case in both axis
  - FCI limit with simple basis sets still are beyond current CC capabilities
  - N e^- require 2^N distinct states – e.g., Benzene N=42, ~4e12 complex numbers
- Density Functional Theory (DFT) proposed to alleviate scaling issues
  - Assumption e^- don't interact
  - Limited accuracy insufficient for several systems of interest
- Possible advantage from QC in representing 2^N wave function of FCI using N qubits





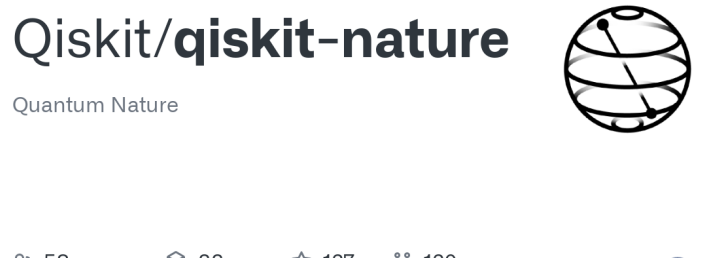
Computational Chemistry and Molecular Simulation

Workflow to compute thermodynamic properties and kinetic rate constants

1. **Compute ground state electronic energy**
2. **Construct potential energy surface (PES)**
   - Compute electronic energy for multiple geometries
3. **Compute vibrational modes of system**
   - Usually through solution of vibrational Schrödinger eq.
   - Approximated with harmonic oscillators
4. **Compute electronic partition function**
   - Thermodynamic properties computable from partition function
   - Kinetic rates require PES for reactants, products, and their transition state (saddle point of PES of reactants and products)

QC has the potential of improving the performance of this three key steps

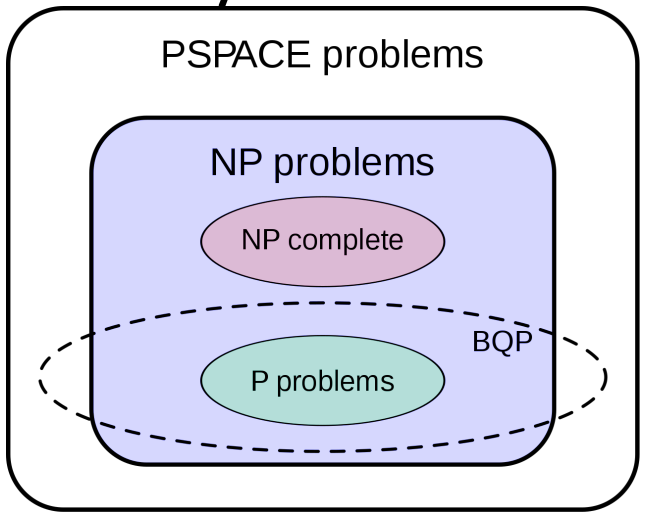
Developed Software workflows addressing these process, e.g.,



Retrieved from github.com/Qiskit/qiskit-nature

Optimization

- **Optimization problems are ubiquitous in science and engineering**
  - Chemical Engineering has been a source of problem and algorithms for the wider community given the issues we encounter
- **Many of these optimization problems cannot be solved "efficiently"**
  - I.e., belong to NP-complete or NP-Hard complexity classes
  - Exponential speedups are believed as unreachable
    - Given application we still are encouraged to develop solution methods
- **QC can provide asymptotic speedup for certain optimization problems**
  - Hard to predict scale at which this is observable
  - **No quantum advantage for practical optimization yet observed**
  - Practical and heuristic speedups are of interest!

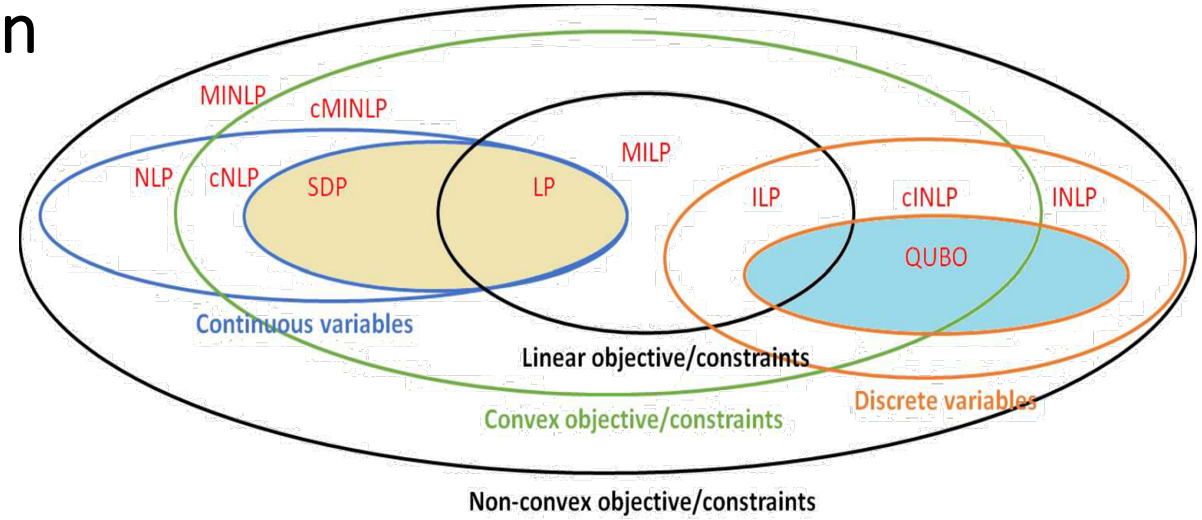


The suspected relationship of BQP to other problem spaces

Retrieved from Michael Nielsen and Isaac Chuang (2000). Quantum Computation and Quantum Information

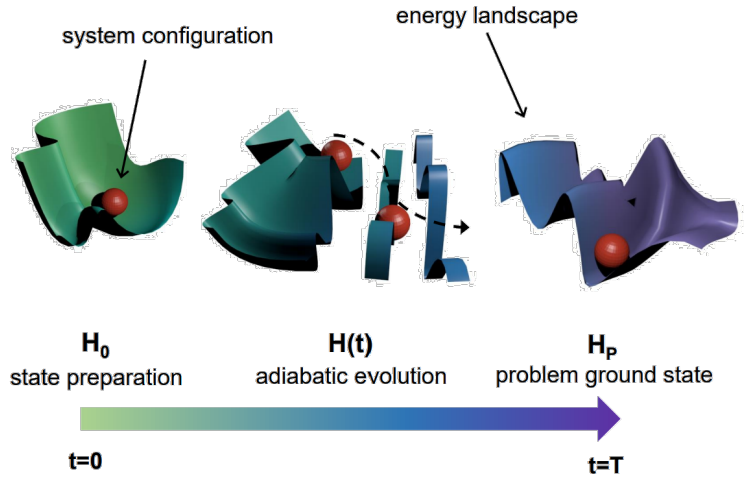
Optimization

- **Optimization problems presented from a mathematical programming perspective**
  - Classified according to objective/constraints linearity/convexity and variables discreteness
- **Proposed algorithms with provable speedup for convex problems (LP/SDP)**
  - Most rely on Q Fourier transform, Q phase estimation, qRAM – Beyond NISQ capabilities
- **Heuristic methods for discrete optimization**
  - Performance bounded by complexity results
    - Unachievable exponential speedup
    - Complete enumeration quadratically faster via Grover search
    - Possible exploitation of structure in the problems
  - Several methods devised for Ising model ↔ Quadratic Unconstrained Binary Opt (QUBO)



Optimization

- **Quantum Adiabatic Algorithm (QAA) proposed for discrete optimization**
  - Adiabatic evolution preserves energy ranking of states
  - Start evolution from system at ground-state
  - Evolve system adiabatically to one that encodes optimization problem
- **Quantum Annealing**
  - Physical implementation of idealized QAA
  - Heuristic method from optimization perspective
- **Myriad of physical or physics-inspired methods**
  - Coherent Ising Machines, Simulated Bifurcation Machines, Digital annealers, …



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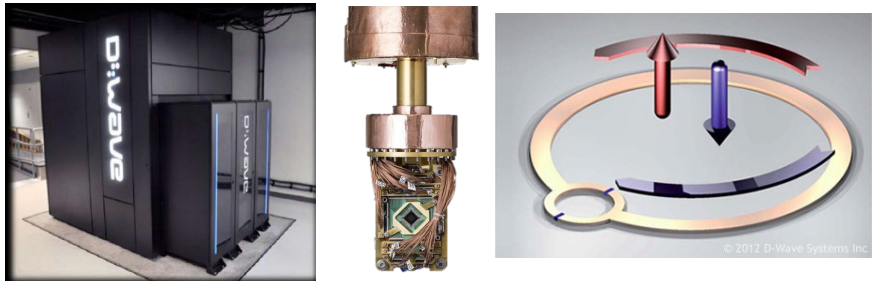

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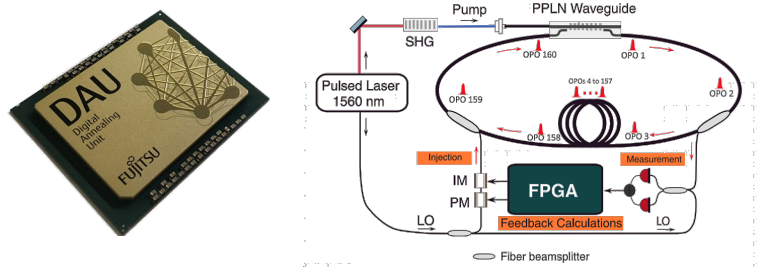


Retrieved from 10.1109/MSPEC.2018.8389173 and DOI: 10.1126/science.aah5178

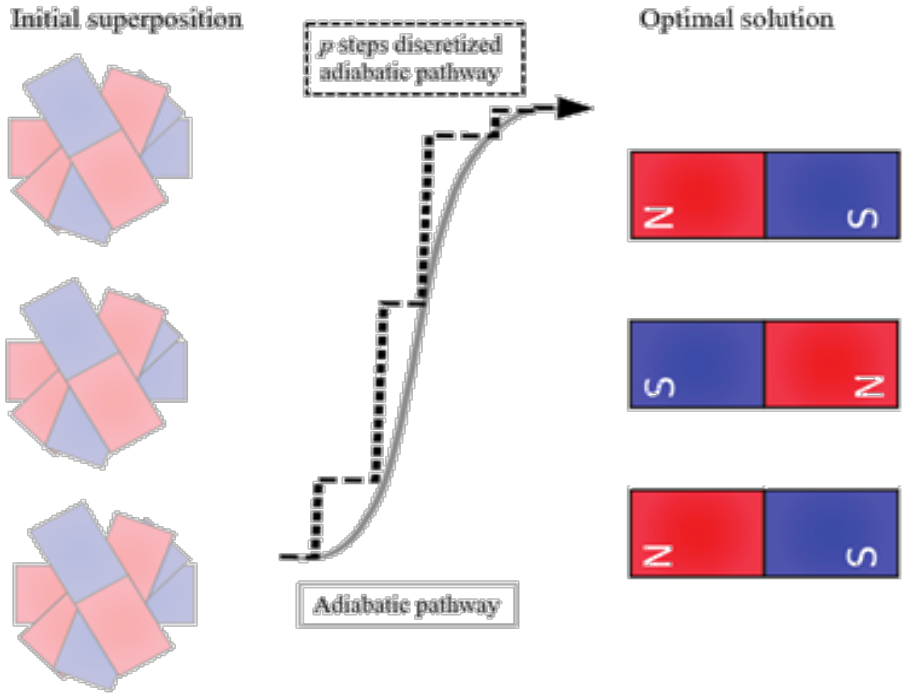
Optimization

- Quantum algorithm to solve discrete optimization problems

1. Map the optimization problem to QUBO/Ising
2. Assign variable in QUBO/Ising to a qubit in a system.
3. Apply a circuit, aiming to maximize the probability of measuring the optimal solution of the problem.
4. Measure the state with output as qubit values.
   - These values yield the optimal solution with some probability
5. Repeat this procedure several times and return the best-found solution

Proposal: Quantum Alternating Optimization Ansatz (QAOA)

- Variational algorithm with Ansatz coming from the QUBO mapping of the problem and the initial state of QAA



Machine Learning

- **Learning patterns from data has become a useful paradigm in science and engineering**
  - ChemE is not the exception with a growing interest in Machine Learning (ML)
- **Observed quantum advantage in different ML tasks motivate looking into it**
  - Learning parity with noise, by IBM in 2017[1]
  - Learning from experiments gathered from quantum sensors, by Caltech in 2021[2]
- **Classification of relevant advances of QC in ML using learning task, realization is near-term devices or requiring fault-tolerance devices, and technology involved in it.**

Near term

	Supervised learning	Unsupervised learning	Reinforcement learning
Quantum annealing	Regularized Regression[98,99]	Boltzmann machine[100]	Reinforcement quantum annealing[101]
Feature embedding	Variational quantum classifier[102] Quantum k-nearest neighbors[103] Quantum enhanced SVM[104]	Quantum k-means[105] Quantum autoencoders[106]	–
Parameterized quantum circuit	Quantum CNNs[107]	Quantum GANs[108,109] Variational Boltzmann machine[110]	Quantum agents[111,112]

Fault tolerant

	Supervised learning	Unsupervised learning	Reinforcement learning
Quantum linear algebra	Least squares regression[113] qSVM[114] Gaussian process[115]	Quantum PCA[116]	–
Grover's search	Quantum k-Nearest Neighbors[103]	Quantum k-medians[117] Quantum k-means[105]	Quantum Reinforcement Learning[118]

1. doi.org/10.1038/s41534-017-0017-3
2. doi.org/10.48550/arXiv.2112.00778

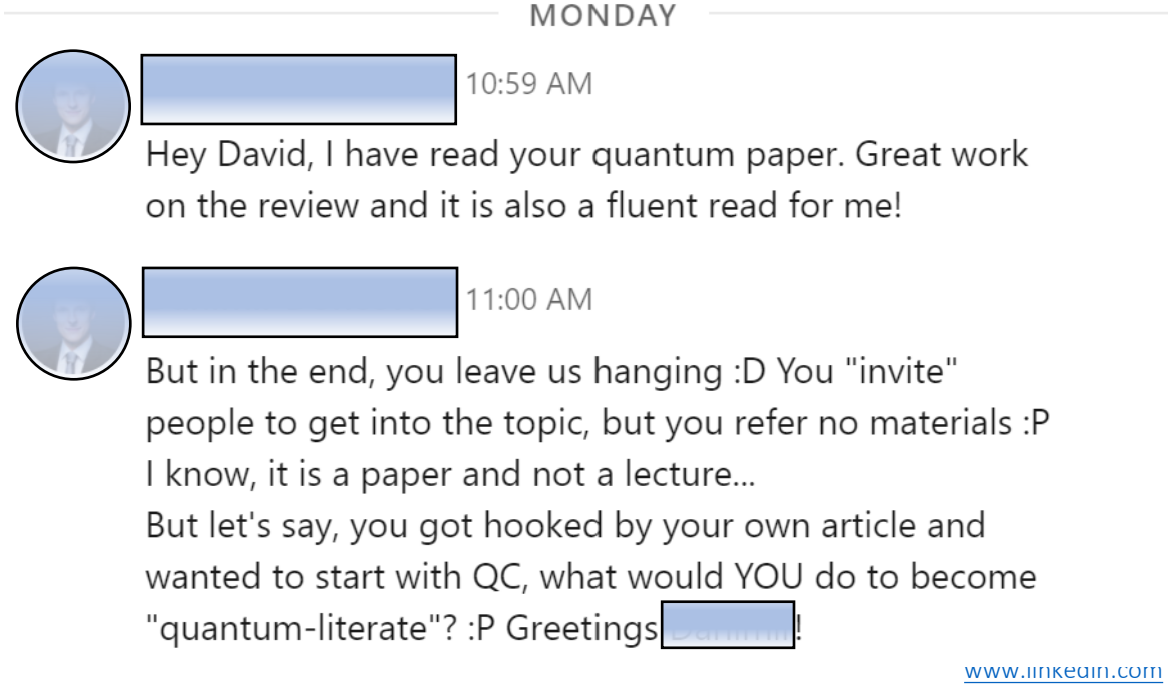
Conclusions and open questions

Current state of QC leads us to identify 3 areas for ChemE with potential quantum advantage

- Computational Chemistry →
  - Although potential, there are still challenges to overcome
  - Current size limitations will only allow for small molecules to be tackled
  - The QM calculations are just part of the workflow, we need to address it all
- Optimization →
  - Complexity of discrete optimization bounds the quantum advantage to practical improvements although not exponential
- Machine Learning →
  - The data feeding and extraction delineates how to better make use for QC

Conclusions and open questions

- Invitation for our community to contribute to the development in QC
- ChemE training useful to tackle several of the great challenges in the area
  - We can serve a big service to create a "quantum-ready workforce"



- Invitation to us in this Workshop: How about if we generate the content that our community needs to "jump into" Quantum Computing?

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Full paper

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