Overview of Quantum Computing and applications in Chemical and Pharmaceutical Engineering

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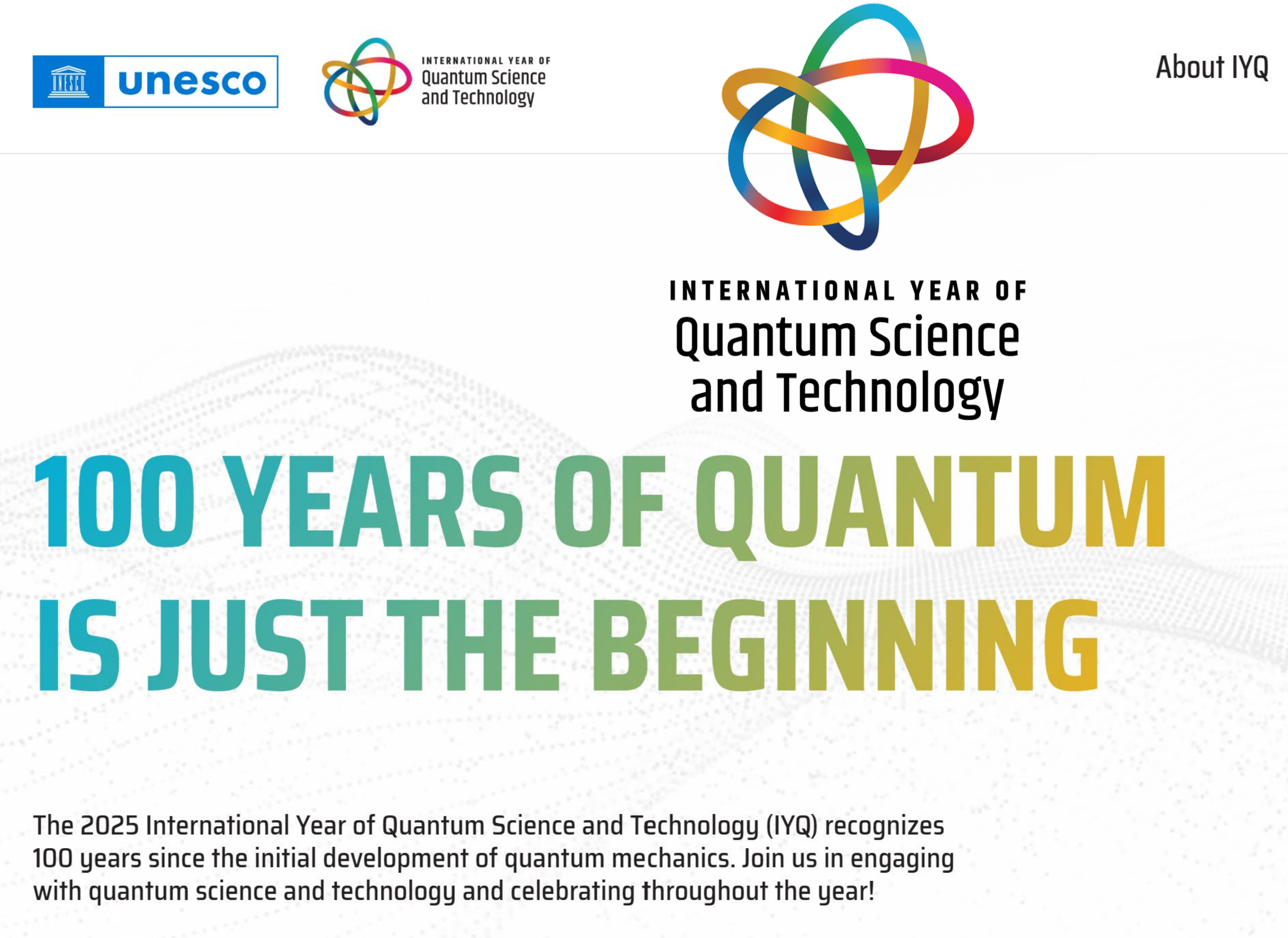
May 8th, 2025

Happy New (Quantum) Year!

According to the UN!



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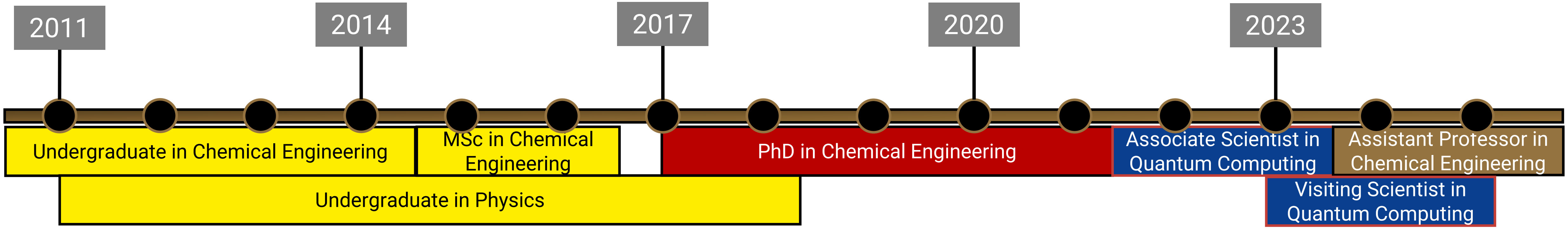
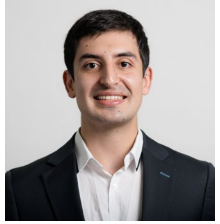


SECQUOIA

Systems Engineering via Classical and Quantum Optimization for Industrial Applications


PI David E. Bernal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Water Processes opt


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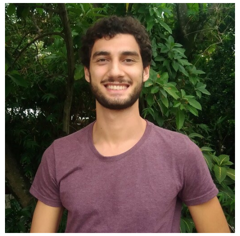
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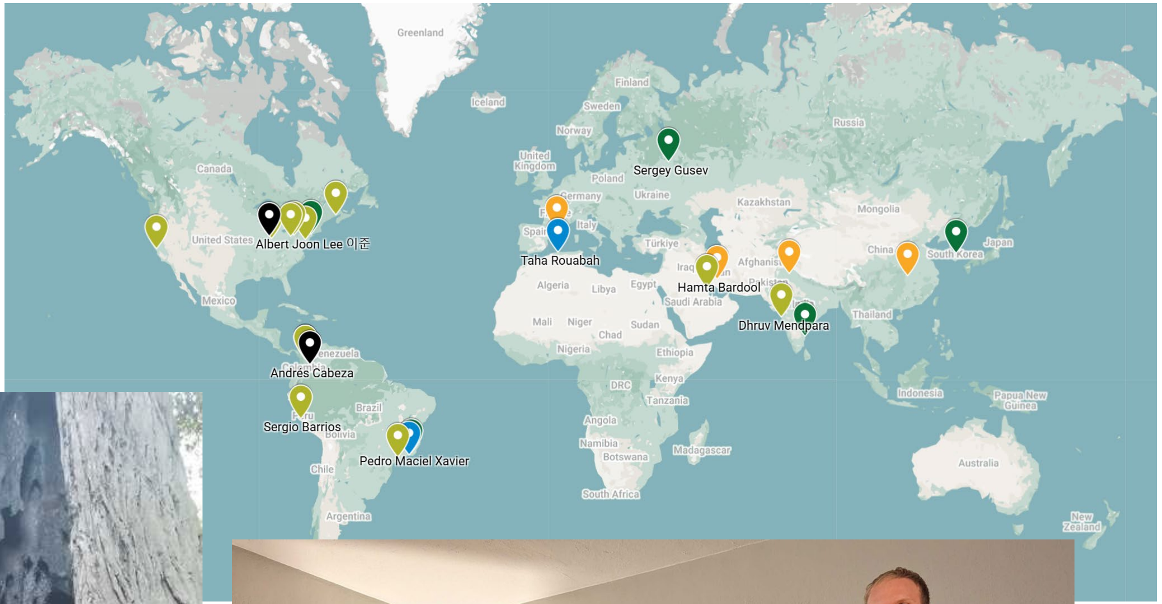
Tensor Networks




PhD Albert Lee
Process Superstructure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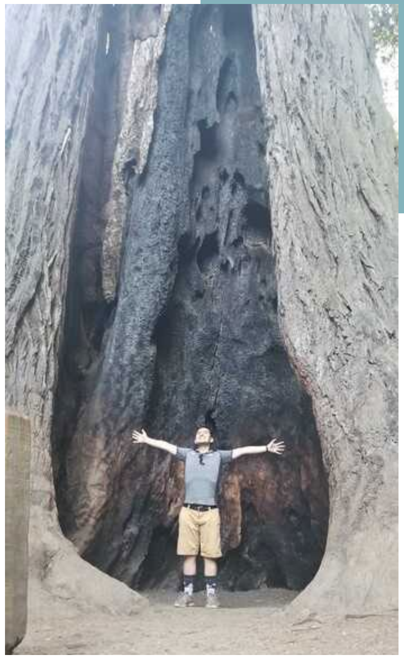
Quantum for Pharma


PhD Anurag Ramesh
Benchmarking Quantum




PhD Pedro Maciel Xavier
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PhD Sergey Gusev
Quantum Conic opt


PhD Andres Cabeza
Process Synthesis

QUANTUM COMPUTING IN CHEMICAL ENGINEERING

PERSPECTIVES ARTICLE AS INVITED CONTRIBUTION

AIChE JOURNAL — An Official Publication of the American Institute of Chemical Engineers — AIChE

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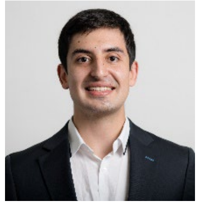
Perspectives of quantum computing for chemical engineering

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

First published: 25 February 2022 | https://doi.org/10.1002/aic.17651



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Carnegie Mellon University
Cornell University Founded A.D. 1865



ExxonMobil Research and Engineering

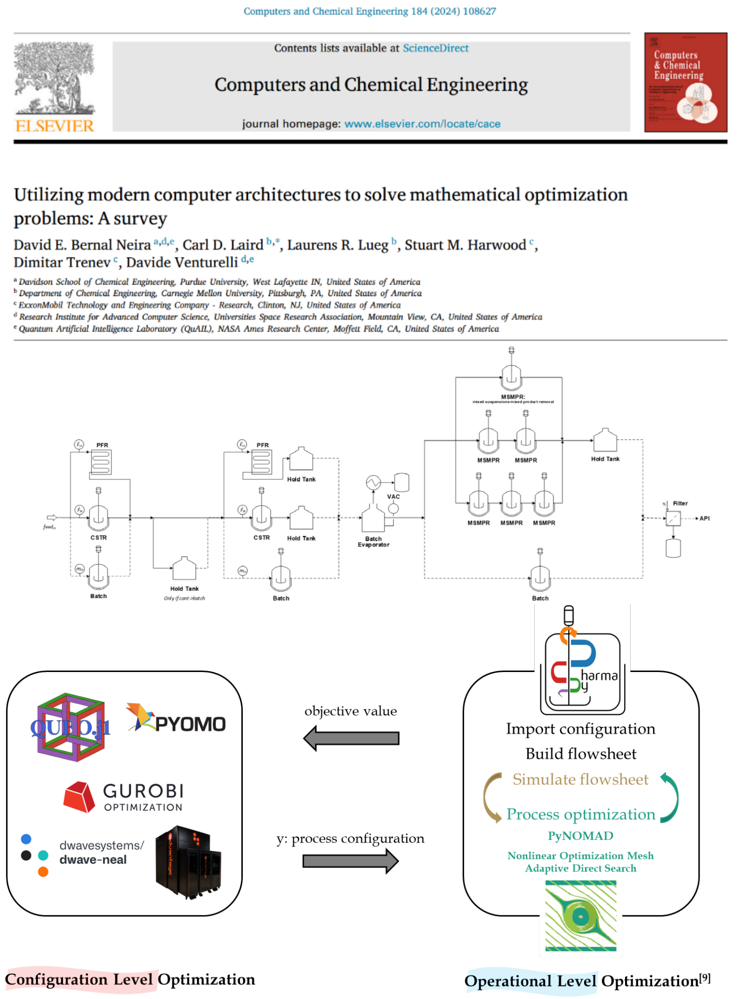
Current state of Quantum Computing leads us to identify **3 areas for ChemE with potential quantum advantage**

- Computational Chemistry
- Optimization
- Machine Learning

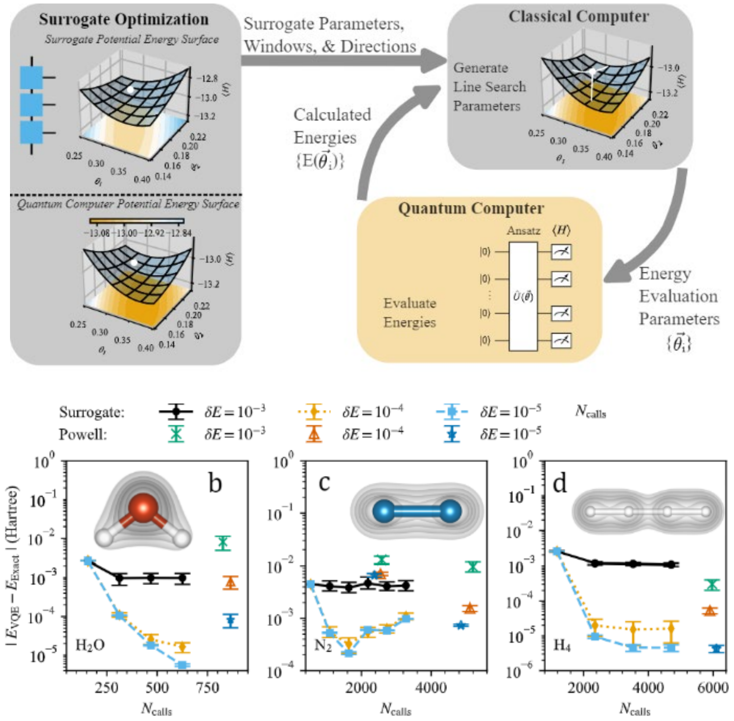
Although potential, there are still challenges to overcome

Hybrid quantum classical research

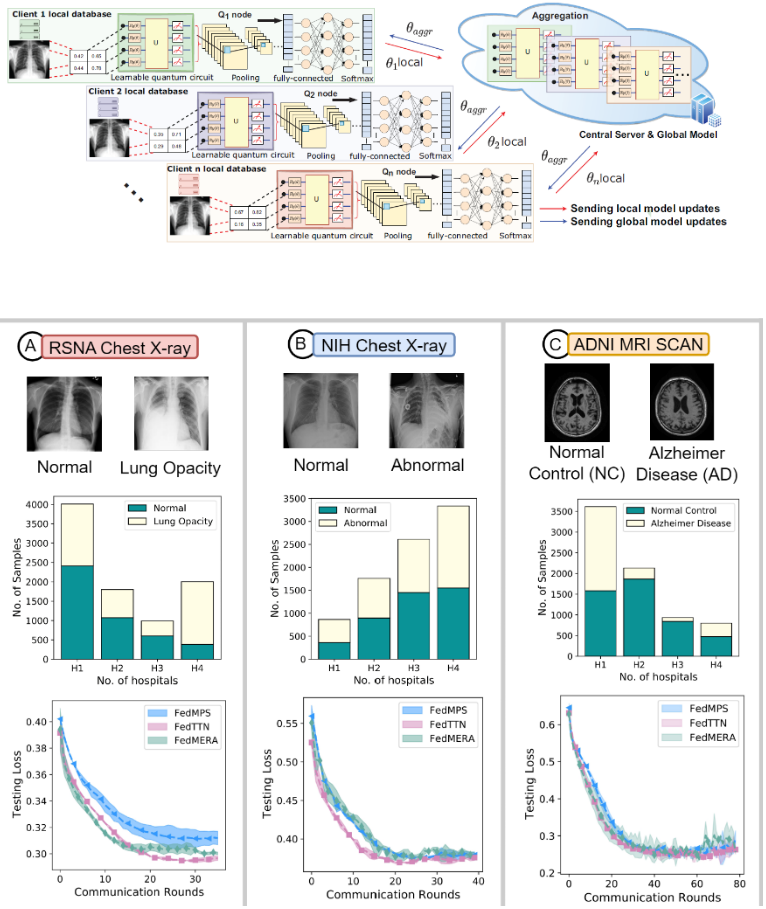
Optimization [1]



Computational Chemistry [2]



Machine Learning



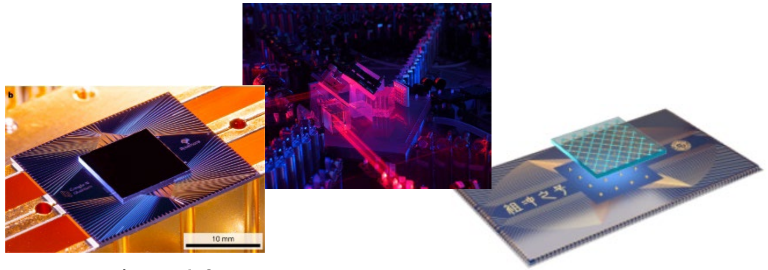
1. Bernal Neira, David E., et al. "Utilizing modern computer architectures to solve mathematical optimization problems: A survey." Computers & Chemical Engineering 184 (2024): 108627.

2. Gustafson EJ, Tiihonen J, Chamaki D, Sorourifar F, Mullinax JW, Li AC, Maciejewski FB, Sawaya NP, Krogel JT, Bernal DE, Tubman NM. Surrogate optimization of variational quantum circuits. arXiv preprint arXiv:2404.02951. 2024 Apr 3.

3. Bhatia, A. S., & Neira, D. E. B. (2024). Federated learning with tensor networks: a quantum AI framework for healthcare. Machine Learning: Science and Technology, 5(4), 045035.

Introduction to Quantum Computing

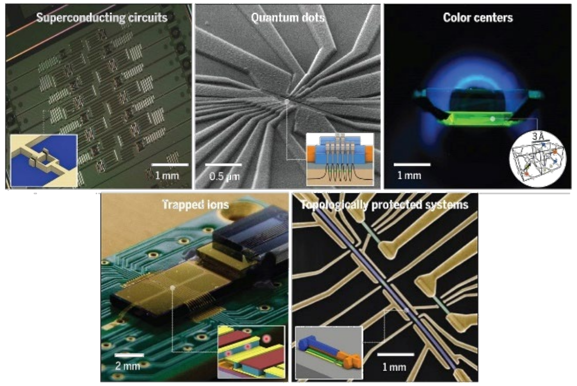
- Practical and functional differences of Quantum Computing (QC) and Classical Computing (CC)
  - Promise to accelerate certain computational tasks
  - Few available experimental evidence of advantage
- Significant progress in algorithms driven by research
  - QC does not extend CC computability, distinction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



Retrieved from doi.org/10.1038/s41586-019-1666-5, doi.org/10.1038/d41586-020-03434-7, doi.org/10.1103/PhysRevLett.127.180501

Quantum Algorithm Zoo

Retrieved from Quantum Algorithm Zoo quantumalgorithmzoo.org/



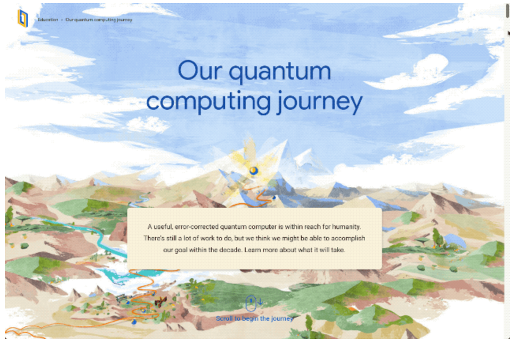
Retrieved from DOI: 10.1126/science.abb2823

qosf

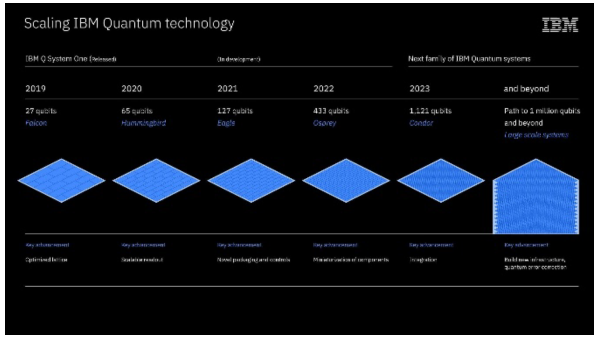
Retrieved from Quantum Open Software Foundation qosf.org/

Introduction to Quantum Computing

- Progress in 40 years but still not achieving “full promise of QC”
- We are living in the Noisy Intermediate Scale Quantum (NISQ) devices era
  - Moderate size (~100s 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 (?)



Retrieved from quantumai.google/learn/map

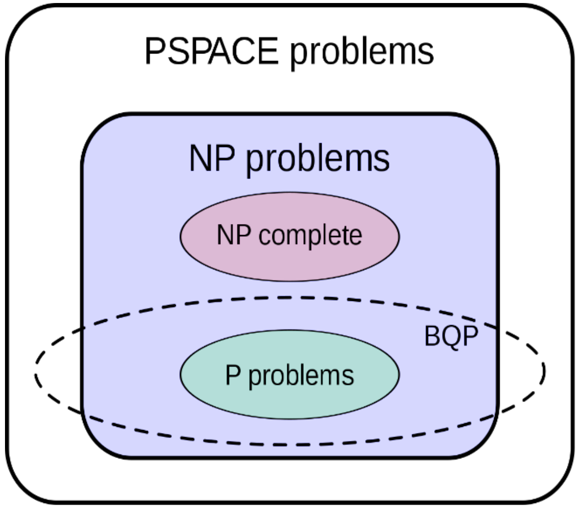


Retrieved from research.ibm.com/blog/ibm-quantum-roadmap

- 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***

Optimization via Quantum Computing

- Optimization problems are ubiquitous in science and engineering
  - ChemE 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 want 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

Flowsheet Optimization using Classical and Quantum Methods in Pharmaceutical Applications

Yirang Park

PURDUE UNIVERSITY | News

Purdue, Heartland BioWorks partners secure $51M in federal funding for regional tech hub

Funding will energize workforce development and startup efforts in biomanufacturing industry

Yirang Park, a Purdue University trainee, prepares a sample of vials for characterization in a lyophilization facility at Discovery Park District at Purdue. (Purdue University photo)

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Award Number (FAIN): 2132142

Managing Division Abbreviation: EFMA **Amendment Number:** 001

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Recipient (Legal Business Name): PURDUE UNIVERSITY
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Official Recipient Email Address: awards@purdue.edu
Unique Entity Identifier (UEI): YRXVL4JYCEF5

AMENDMENT INFORMATION

Amendment Type: Supplement
Amendment Date: 08/08/2023
Amendment Number: 001
Proposal Number: 2234175
Amendment Description:

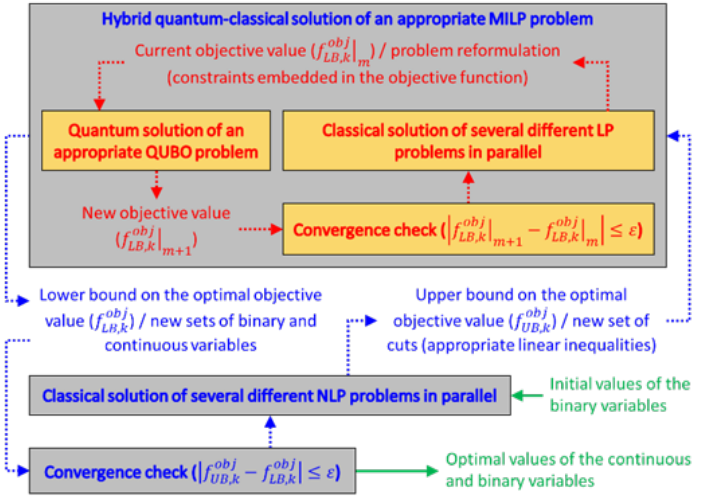


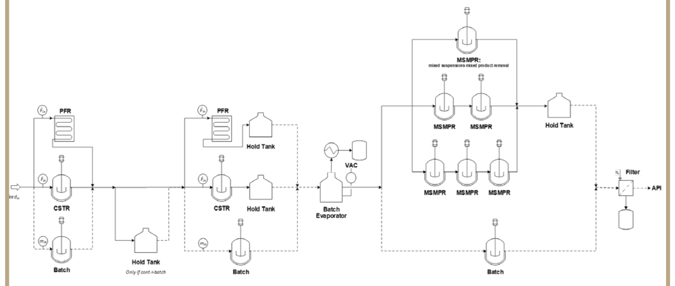
Figure 1: Overview of the proposed QUBO outer approximation (QOA) algorithm (green text – input and output data; blue text – outer approximation steps; red text –hybrid, quantum-classical strategy for solving QOA's MILP problem).

Table 1: Principal optimization problems included in the project, organized by Specific Aim.

Specific Aim	Optimization Problems
1 – Discovery of new flow synthesis routes and processes for Imatinib and Lisinopril, using machine learning and high-throughput experimentation.	Identification of optimal, initial DoE's for both test drugs, using optimization-driven, space-filling DoE strategies [NLP*]; Discovery of new reaction pathways for both test drugs by integer optimization, using the machine learning model as a black-box simulator [MIP*].
2 – Robust digital design and optimal real-time operation of modular mini-plants for distributed drug manufacturing	Definition of optimal flowsheet structure, process unit sizes, and steady-state operating conditions for every type of basic mini-plant module [S-MINLP*]; Computation of optimal dynamic operating conditions, including appropriate startup and shutdown procedures, for every type of mini-plant module [S-DO*].
3 – Estimation of optimal, individualized drug administration regimens	Identification of optimal, individualized dosage regimens for both model drugs and a representative set of patients [S-DO*].
5 – Optimal design and operation of new drug supply chain infrastructures	Optimal design of resilient drug supply chain infrastructures for both test drugs [S-MILP*]; Identification of robust supply chain operating procedures, able to cope with unforeseen, highly disruptive events for both test drugs [S-MILP*].

** NLP: nonlinear programming; DO: dynamic optimization; MIP: mixed-integer programming; MILP: mixed-integer linear programming; MINLP: mixed-integer nonlinear programming; S-: stochastic / under uncertainty*

Superstructure-based Optimization



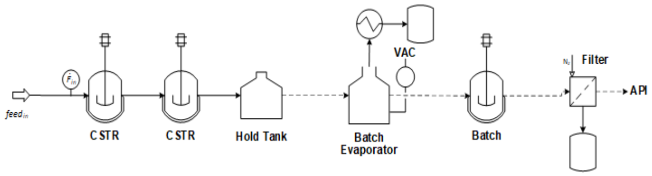
Superstructure

- Single flowsheet to encapsulate all feasible alternative structures
- Represents solution space for process synthesis problem

$$
\begin{aligned}
\min_{x,y}\ & f(x,y) \\
\text{s.t.}\quad & h(x,y) = 0 \\
& g(x,y) \leq 0 \\
& x \in X \subseteq \mathbb{R}^n \\
& y \in Y \subseteq \mathbb{Z}^p
\end{aligned}
$$

Mathematical Programming Formulation

- Formulate the optimization problem as a mathematical programming model



Optimal Solution

- Solve the model via optimization algorithms
- Find the optimal configuration

[4] Tomio Umeda et.al. Chemical Engineering Science, 1972.
[5] G R Kocis and I E Grossmann, *Computers & Chem. Eng.*, 1989.
[6] Metin Türkay and Ignacio E. Grossmann. *Computers & Chemical Engineering,* 1996.
[7] Qi Chen and I. E. Grossmann, *Annual Review of Chemical and Biomolecular Engineering,* 2017.

Method: Optimization Framework

QUBO.jl

PYOMO

GUROBI OPTIMIZATION

dwavesystems/
dwave-neal

objective value

y: process configuration

Import configuration

Build flowsheet

Simulate flowsheet

Process optimization

PyNOMAD

Nonlinear Optimization Mesh Adaptive Direct Search

Configuration Level Optimization

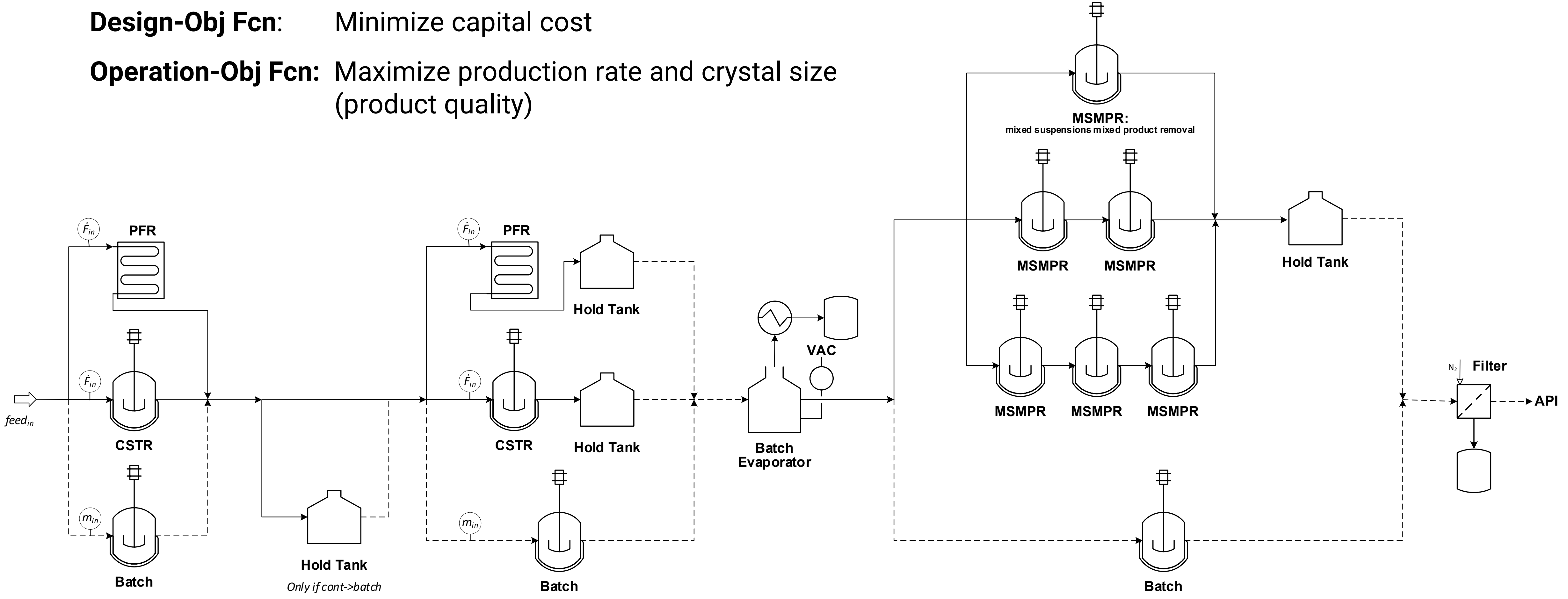
Operational Level Optimization[9]

[9] Yash Barhate et al. *Computer Aided Chemical Engineering*, 2024.
[25] Pedro Maciel Xavier et al. *arXiv: Math*, 2023.
[26] Michael L. Bynum et al. *Springer Science & Business Media*, 2021.
[27] Gurobi Optimization, LLC. Gurobi Optimizer Reference Manual, 2024.
[28] D-Wave Systems Inc. Neal: Simulated Annealing Sampler, 2024.
[29] Daniel Casas-Orozco et al. *Computers & Chemical Engineering*, 2021.
[30] Charles Audet et al. *ACM Trans. Math. Softw.*, 2022.

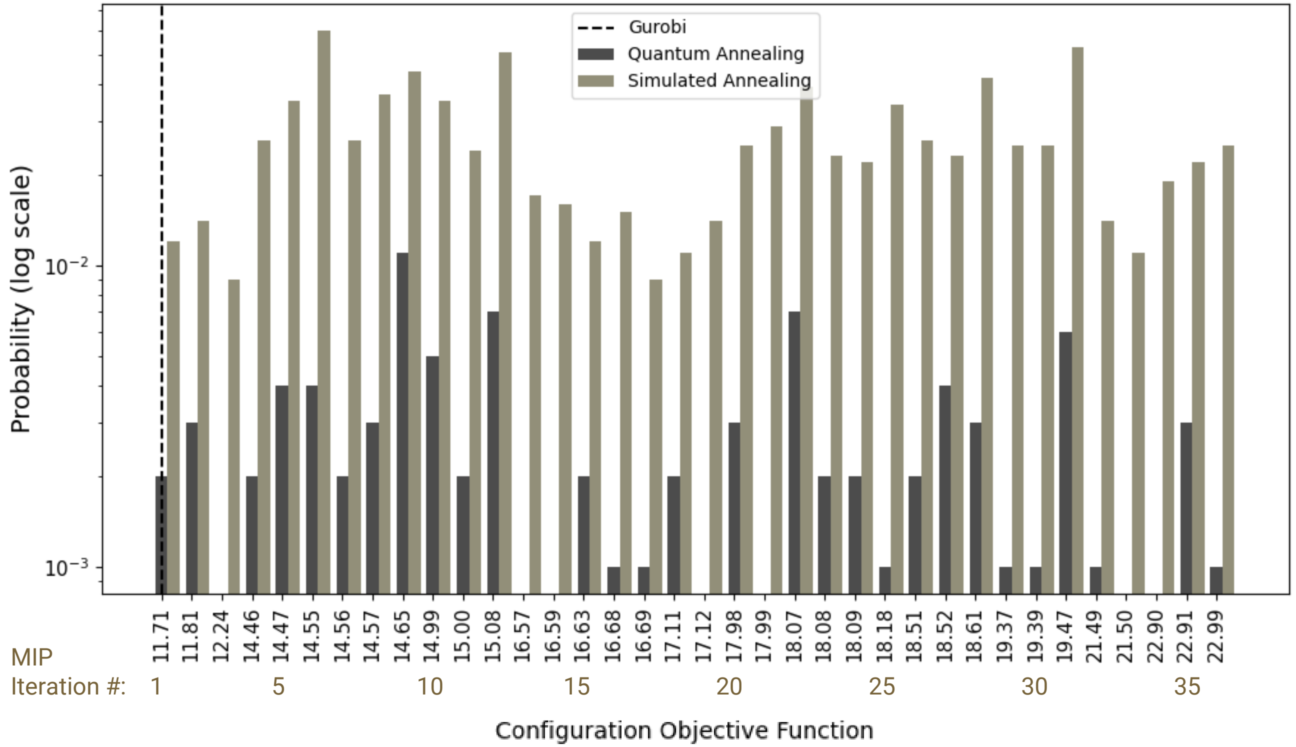
Case Study: Drug Substance Synthesis Process

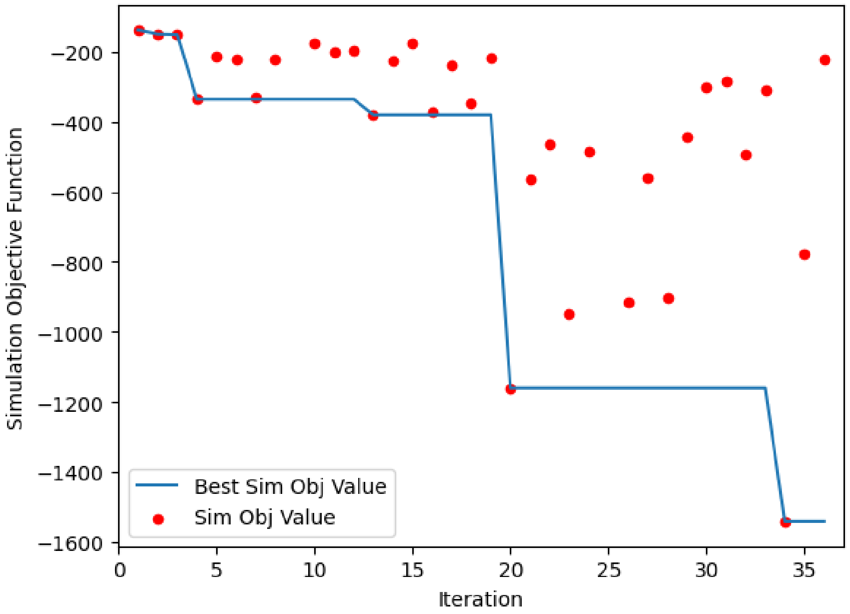
Design-Obj Fcn: Minimize capital cost

Operation-Obj Fcn: Maximize production rate and crystal size (product quality)



Preliminary Results: Simulation Optimization





- Provides a way to evaluate process design level decisions and operational decisions
- Simulation objective value does not improve with configuration decisions
  - Objective functions are **not aligned**

Clinical trial optimization competition

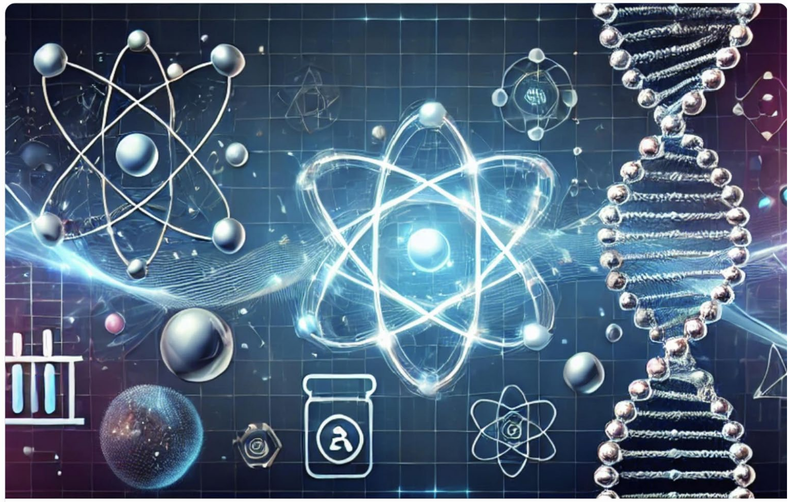
aqora

stubbi • Jan 13, 2025

Advancing Clinical Trial Optimization with Quantum Computing: Ingenii's Competition on Aqora Improves Existing Solutions

3

Explore how Ingenii's quantum competition on Aqora generated pioneering solutions that outperform benchmarks in clinical trial optimization—cutting costs, accelerating R&D, and driving corporate innovation.



Clinical Trial Optimization

Optimize clinical trials based on the Mayo Clinic dataset

Hosted by ingenii

Problem formulation

Putting it all together, this problem can be formulated as follows:

$$\min_x \sum_{s=1}^{3} |\Delta\mu_s| + \rho \sum_{s=1}^{3} |\Delta\sigma_{ss}| + 2\rho \sum_{s=1}^{3} \sum_{s'=s+1}^{3} |\Delta\sigma_{ss'}| = d$$

$$\text{s.t}$$

$$\sum_i x_{ip} = n/2, \quad \forall p \in \{1,2\}$$

$$x_{i1} + x_{i2} = 1, \quad \forall i \in \{1,\cdots,n\}$$

$$x_{12} = 0$$

This corresponds to a mixed-integer optimization problem with 10 continuous variable ($\{d, \Delta\mu_1, \Delta\mu_2, \Delta\mu_3, \Delta\sigma_{11}, \Delta\sigma_{22}, \Delta\sigma_{33}, \Delta\sigma_{12}, \Delta\sigma_{13}, \Delta\sigma_{23}\}$) and $2n-1$ binary variables ($\{x_{11},\cdots,x_{n1},x_{22},\cdots,x_{n2}\}$).

Solving this optimization problem classically is challenging (or even impossible!) when the number of patients is large. For this reason, quantum computing can provide significant advantage to solve this kind of problems.

Key Performance Insights

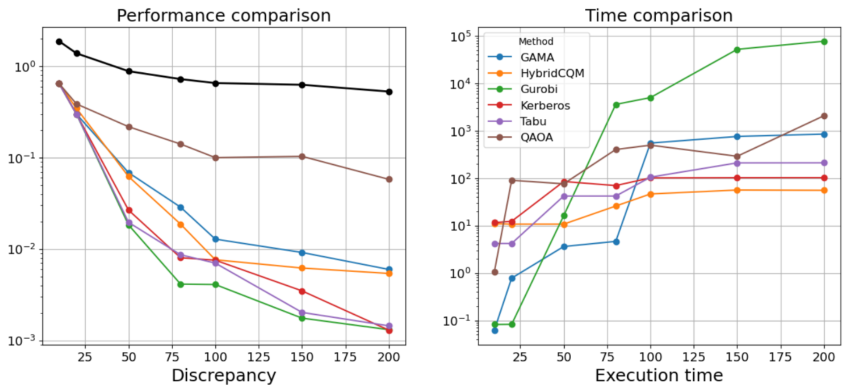


Figure 1: Time and performance comparison of multiple classical, quantum-inspired and hybrid quantum-classical solutions. The black line represents the average discrepancy obtained by random patient stratification.

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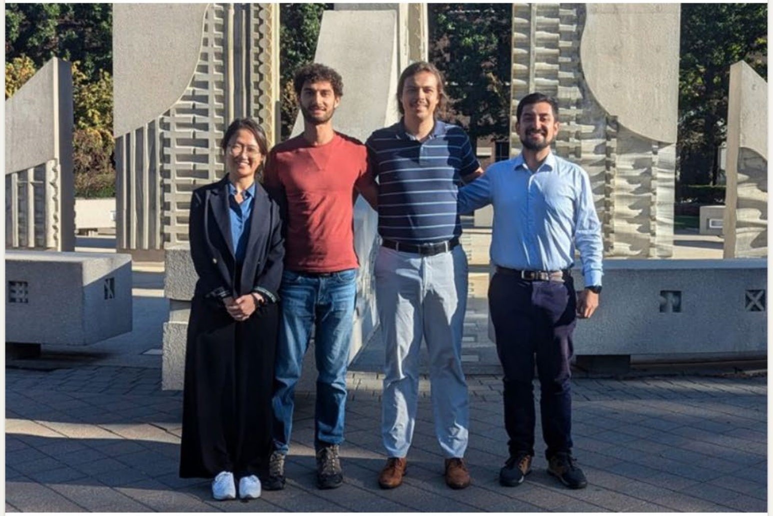
Professor David Esteban Bernal Neira and his research group, SECQUOIA, were recently awarded in the Clinical Trial Optimization Competition.

Their unique approach to solving the proposed quantum computing problem earned them a spot among the top three teams in the world.

Read more about their method and the competition, and watch their presentation on our website: https://lnkd.in/gcvsDCM7

#Purdue #PurdueChE #ChE #QuantumComputing #MayoClinic #Engineering #ChemicalEngineering



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Reactions

+76

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.

McKinsey & Company

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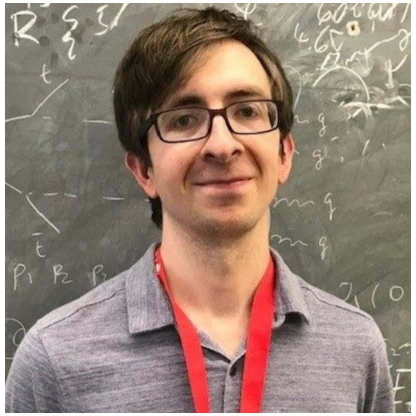
Surrogate Optimization for Variational Quantum Algorithms



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Diana Chamaki

Norm Tubman

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Surrogate Optimization for Variational Quantum Algorithm

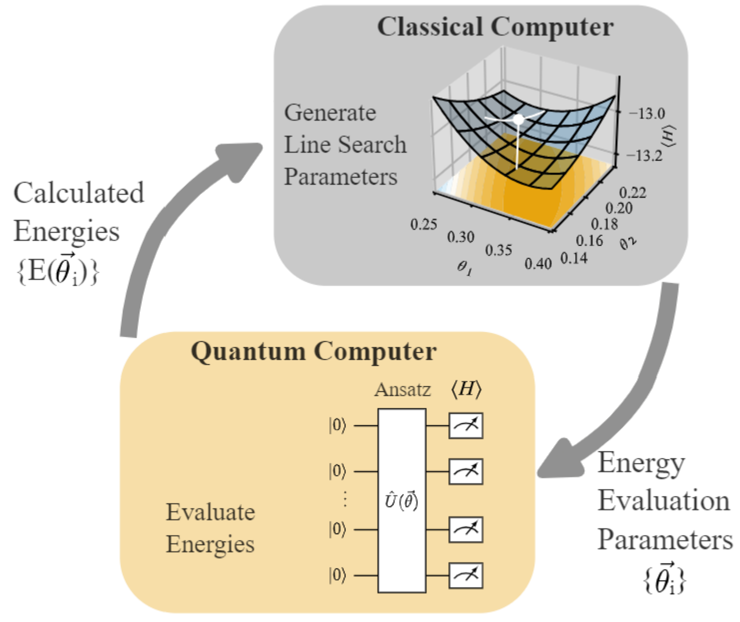


FIG. 1. Diagram of the surrogate line search optimization procedure. The energy surfaces shown correspond to a 2D projection of the energy surface for the Ising model studied in this work. The feedback loop between the classical computer and the quantum processing unit (QPU) or quantum computer repeats for as many iterations as desired.

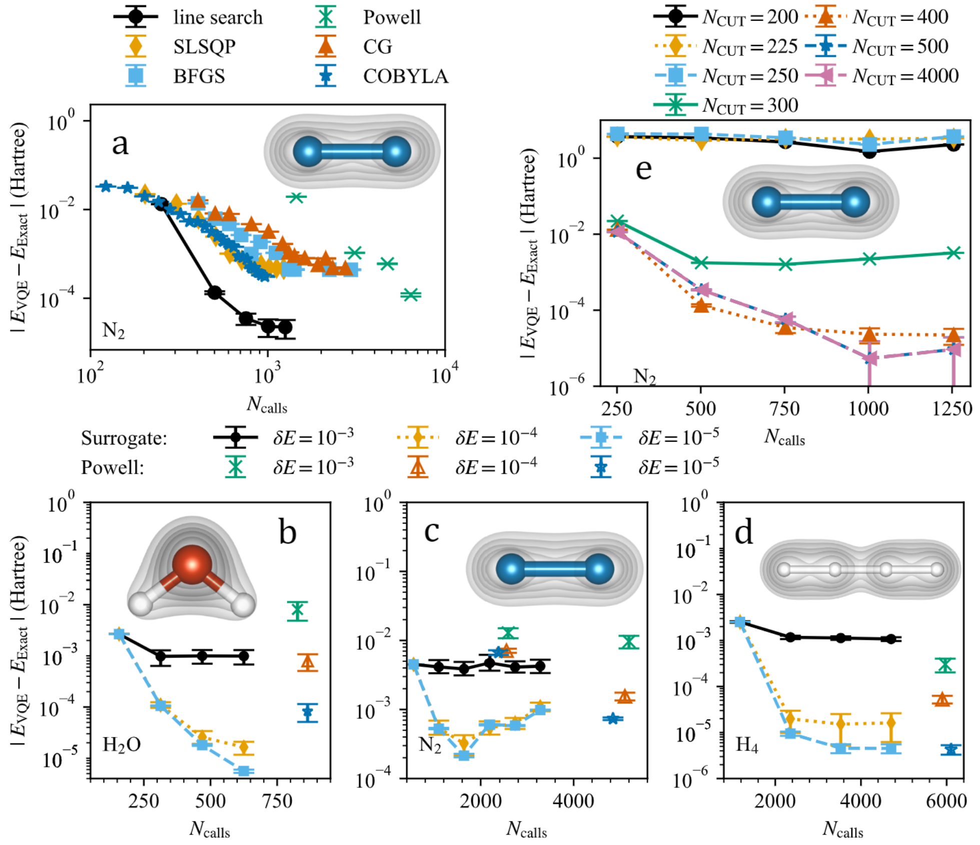


FIG. 2. **a**: A comparison of the performance of surrogate line search, SLSQP, BFGS, Powell, COBYLA, and conjugate gradient (CG) for the N_2 molecule in the cc-pvdz basis using the 18 lowest orbitals and 50 terms from the CCSD expansion with the largest coefficients. The resolution on the energy is $\delta E = 10^{-5}$. **b-d**: Comparison of Powell optimizer to the surrogate line search using 7 points per search direction for three molecules and bases: H_2O in STO-3G basis (left), N_2 in STO-3G basis (middle), H_4 chain in cc-pvdz basis with interatomic distance 1.27Å (right). Solid markers correspond to the surrogate line search, and open markers correspond to the Powell optimizer. The details of each simulation are provided in Table . **e**: Comparison of different values of N_{CUT} for a truncated N_2 simulation using the parameters from Table and energy uncertainties $\delta E = 10^{-5}$.

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, technology involved in it, and realization in near-term devices or requiring fault-tolerance devices.

Near term

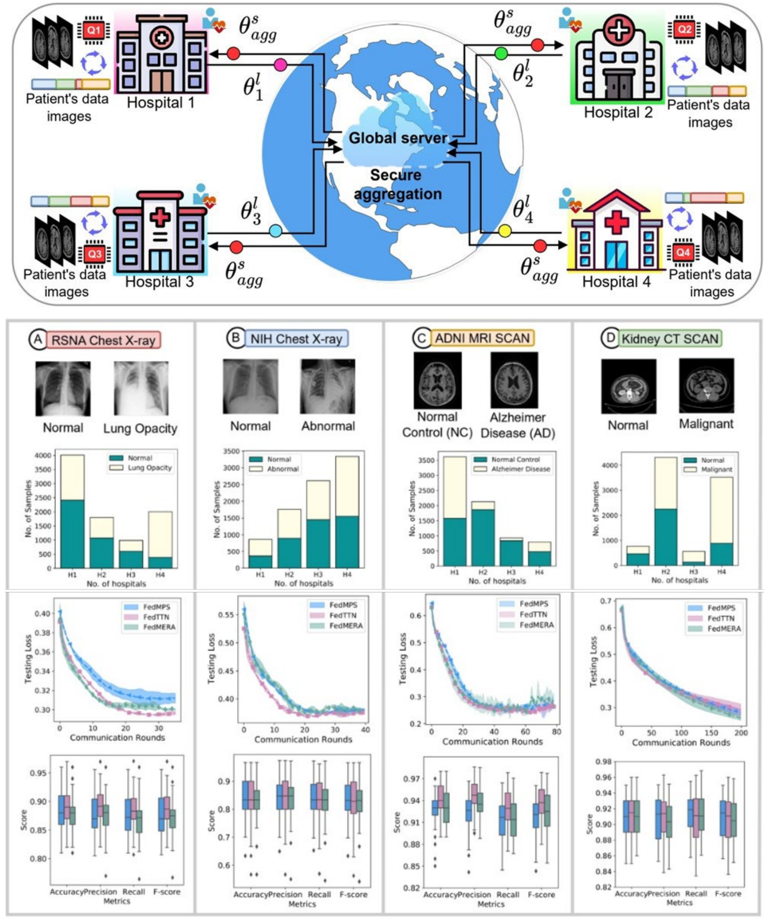
	Supervised learning	Unsupervised learning	Reinforcement learning
Quantum annealing	Regularized Regression [98] [99]	Boltzmann machine [100]	Reinforcement quantum annealing [101]
Feature embedding	Variational quantum classifier [102] Quantum k-nearest neighbors [103] Quantum enhanced SVM [104]	Quantum 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

Federated Learning with tensor networks: a quantum AI framework for healthcare



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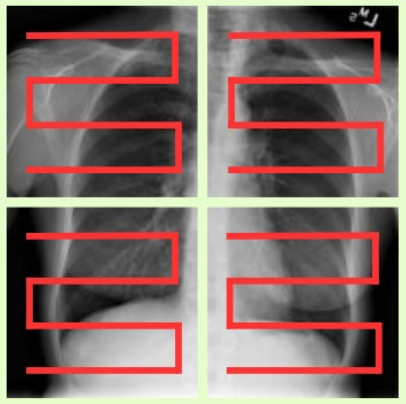
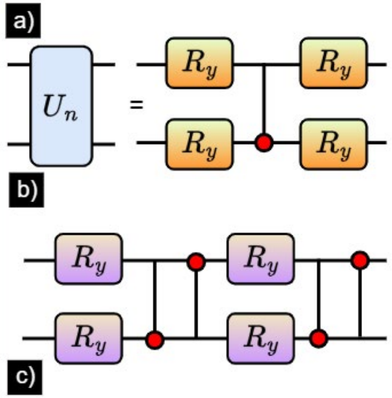
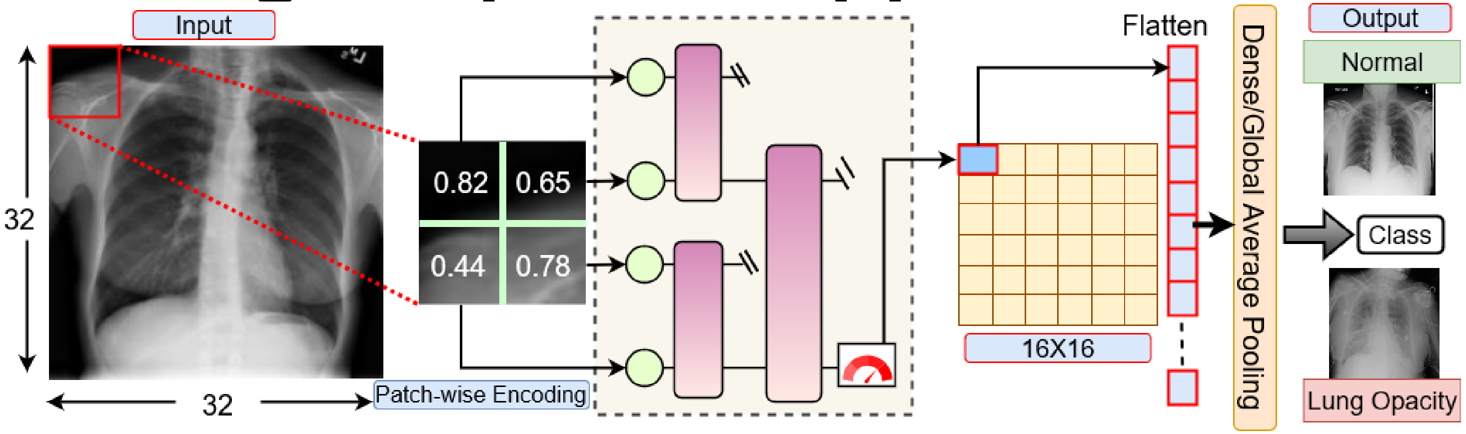
[2]Quantum Artificial Intelligence Laboratory, NASA Ames Research Center

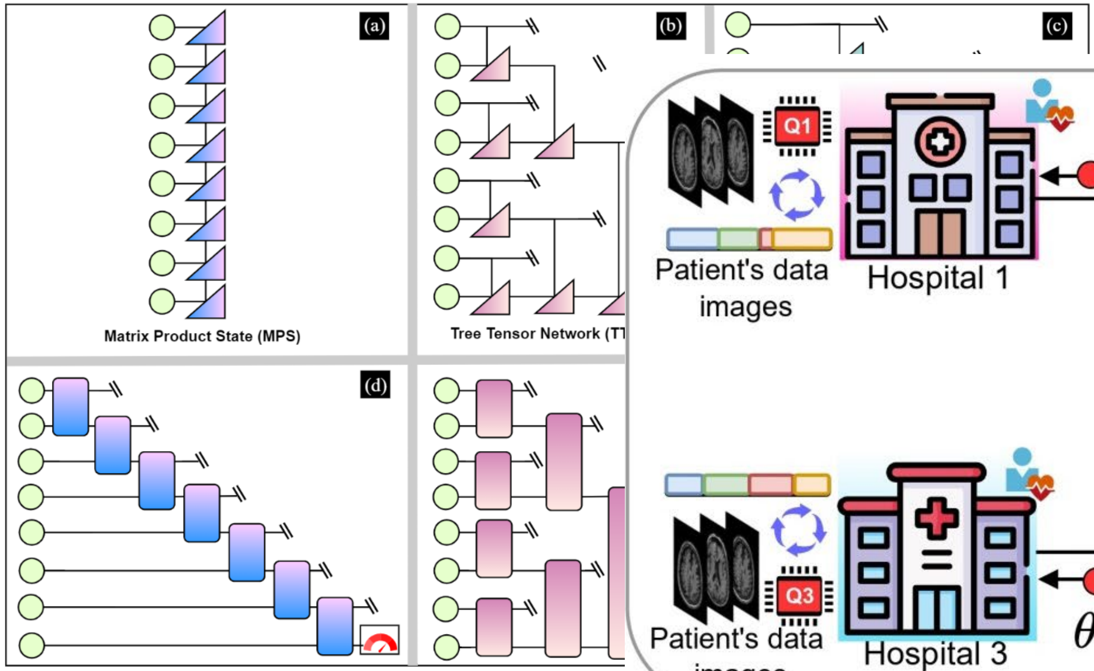
[3]Research Institute of Advanced Computer Science, Universities Space Research Association

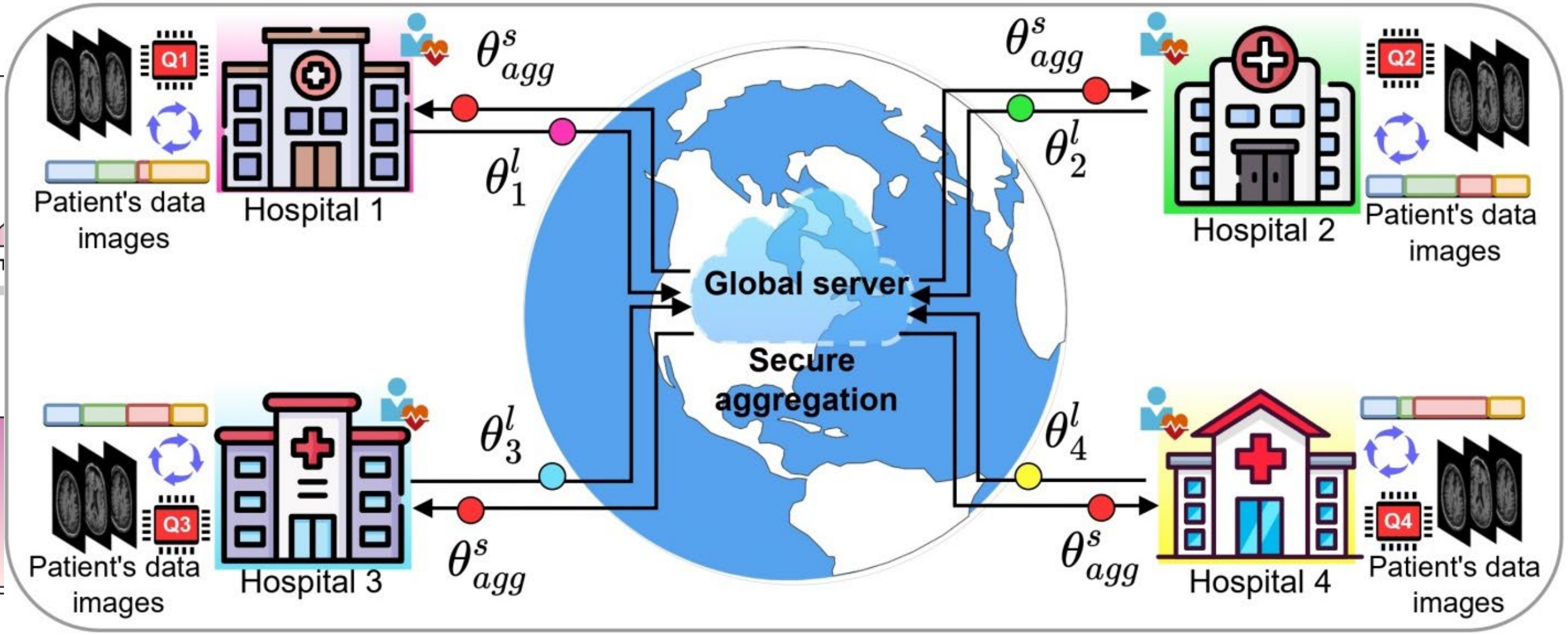
Quantum Federated Learning Proposed Approach



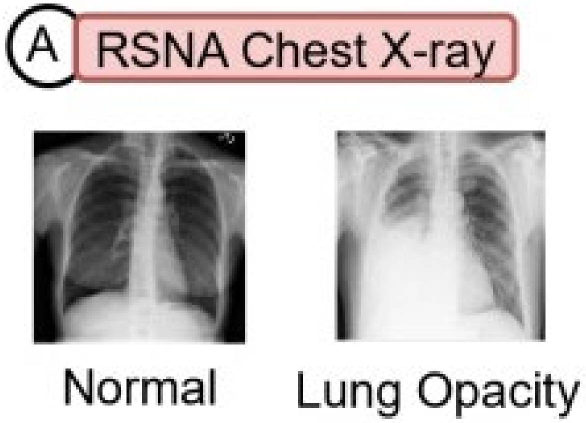


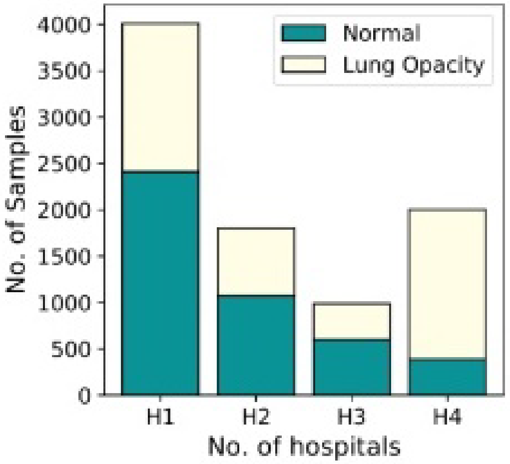


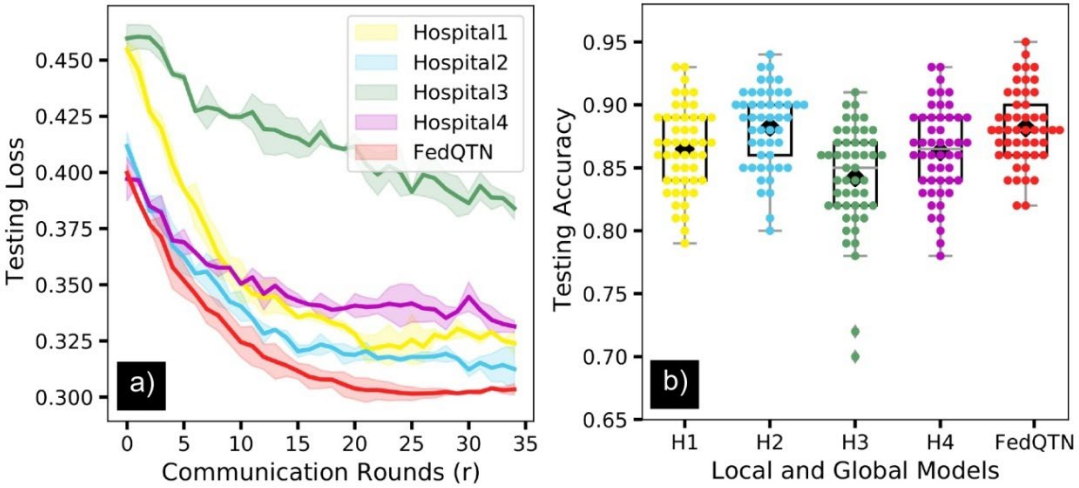


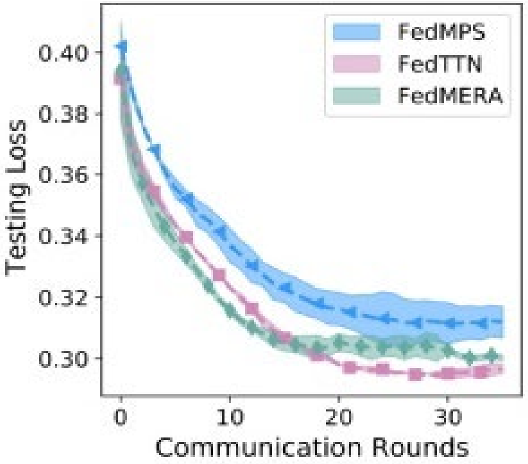


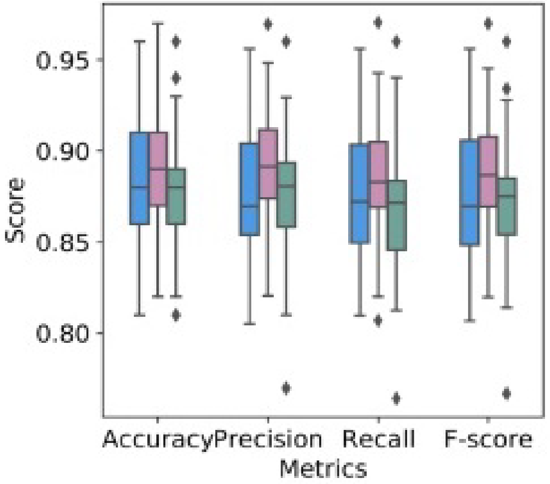
Example Results





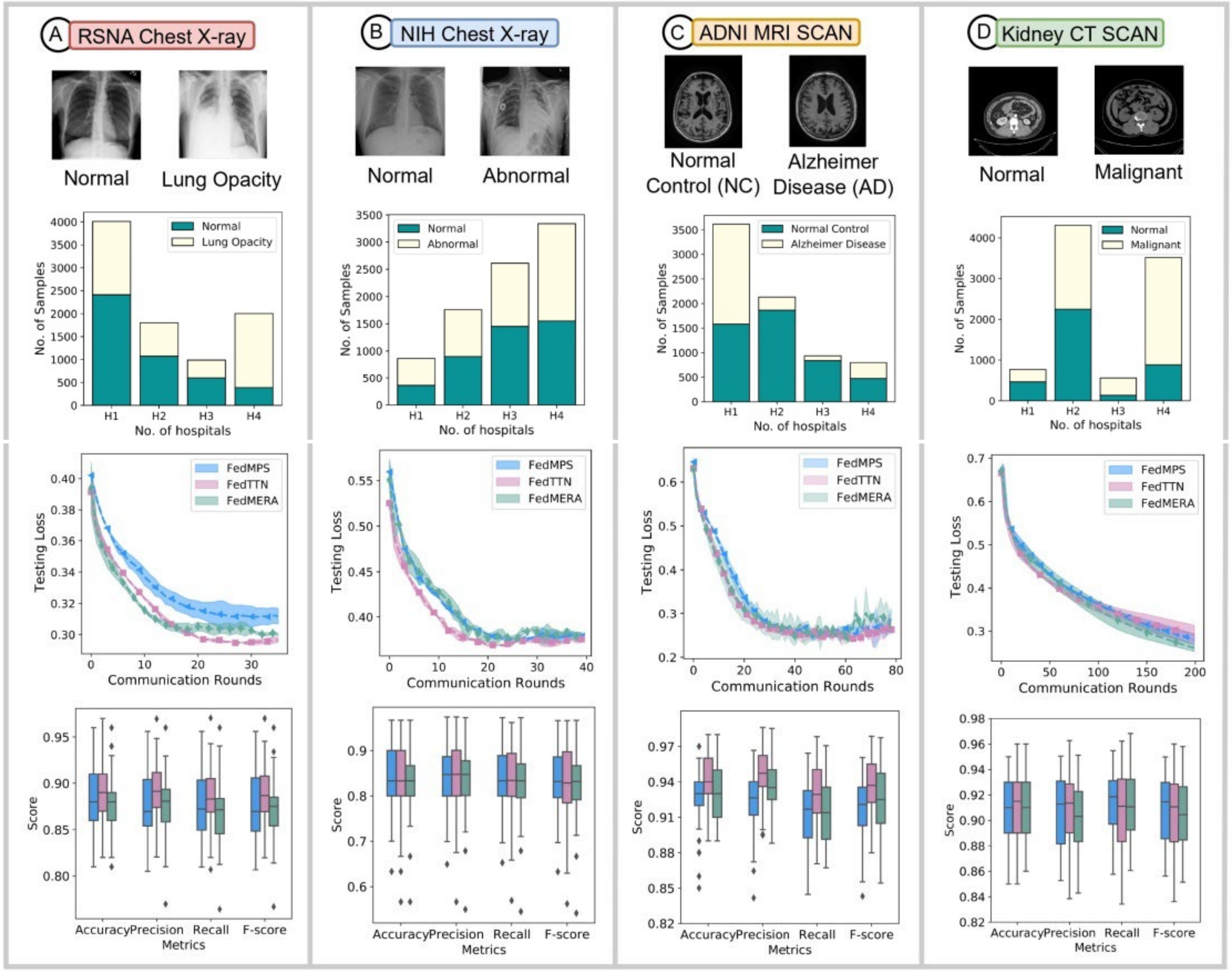


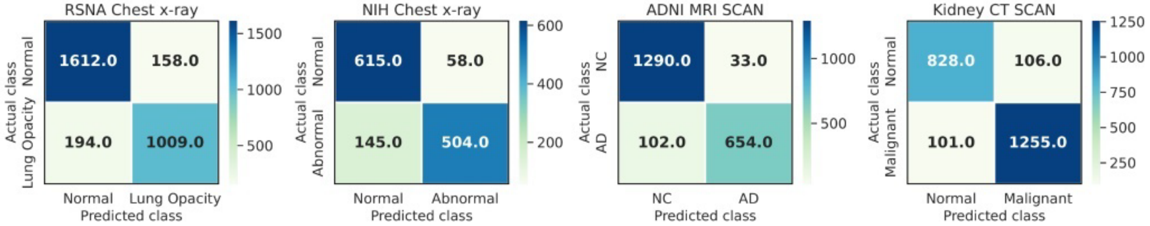


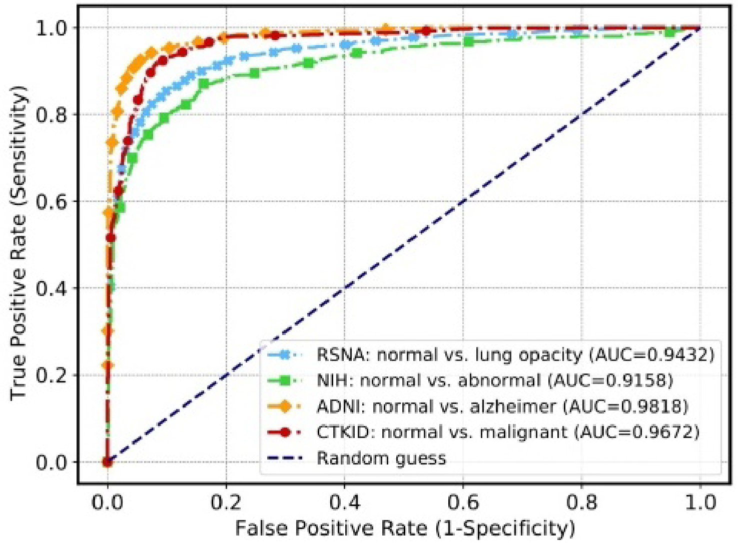


The **FedQTN global model** significantly outperforms individual local models regardless of how uneven and insufficient data distributions are and significantly obtains a **smoother and faster** convergence .

More Examples

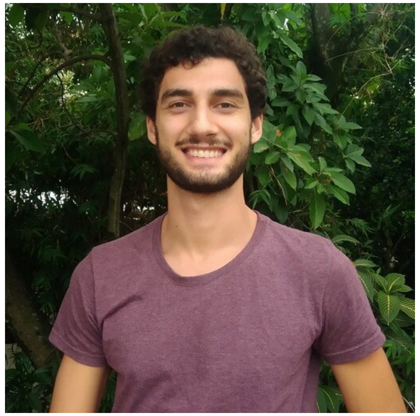






Federated Learning for Chemical Engineering

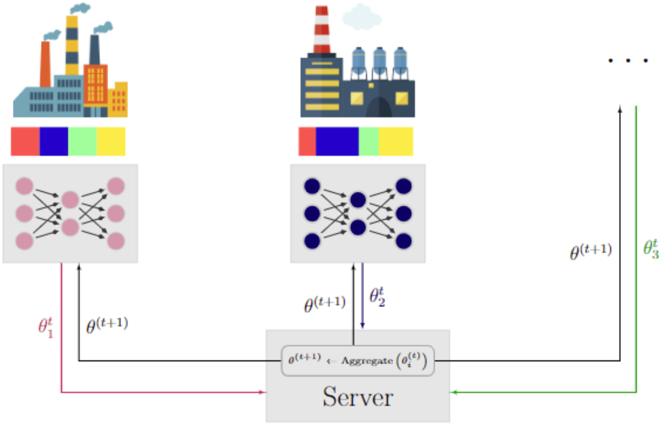
Siddhant Dutta

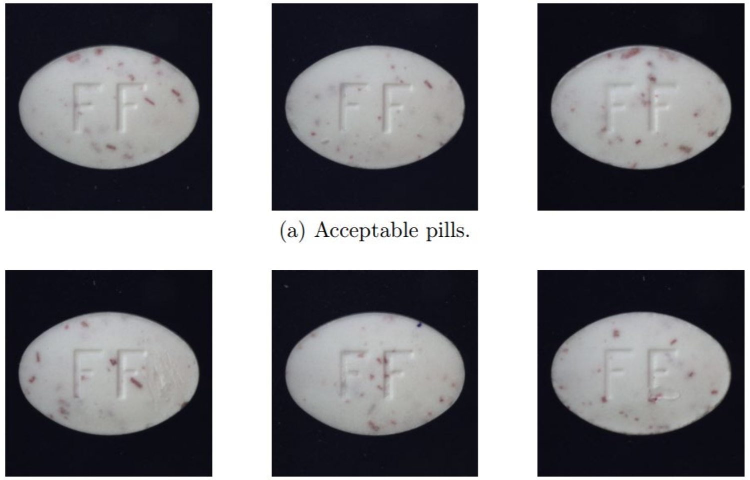


Iago Leal

Claudio Farias

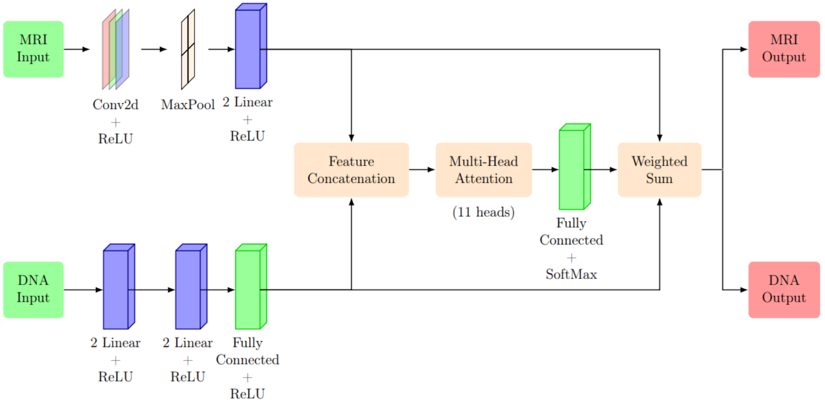
Pedro M. Xavier





(a) Acceptable pills.

(b) Defective pills.



Dutta, Siddhant, et al. "Federated Learning in Chemical Engineering: A Tutorial on a Framework for Privacy-Preserving Collaboration Across Distributed Data Sources." *arXiv preprint arXiv:2411.16737* (2024).

Conclusions and open questions

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

Although potential, there are still challenges to overcome

- Computational Chemistry
  - Current size limitations will only allow for small molecules to be tackled
  - The Q Mechanics 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

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Brief Communication | Open access | Published: 22 January 2025

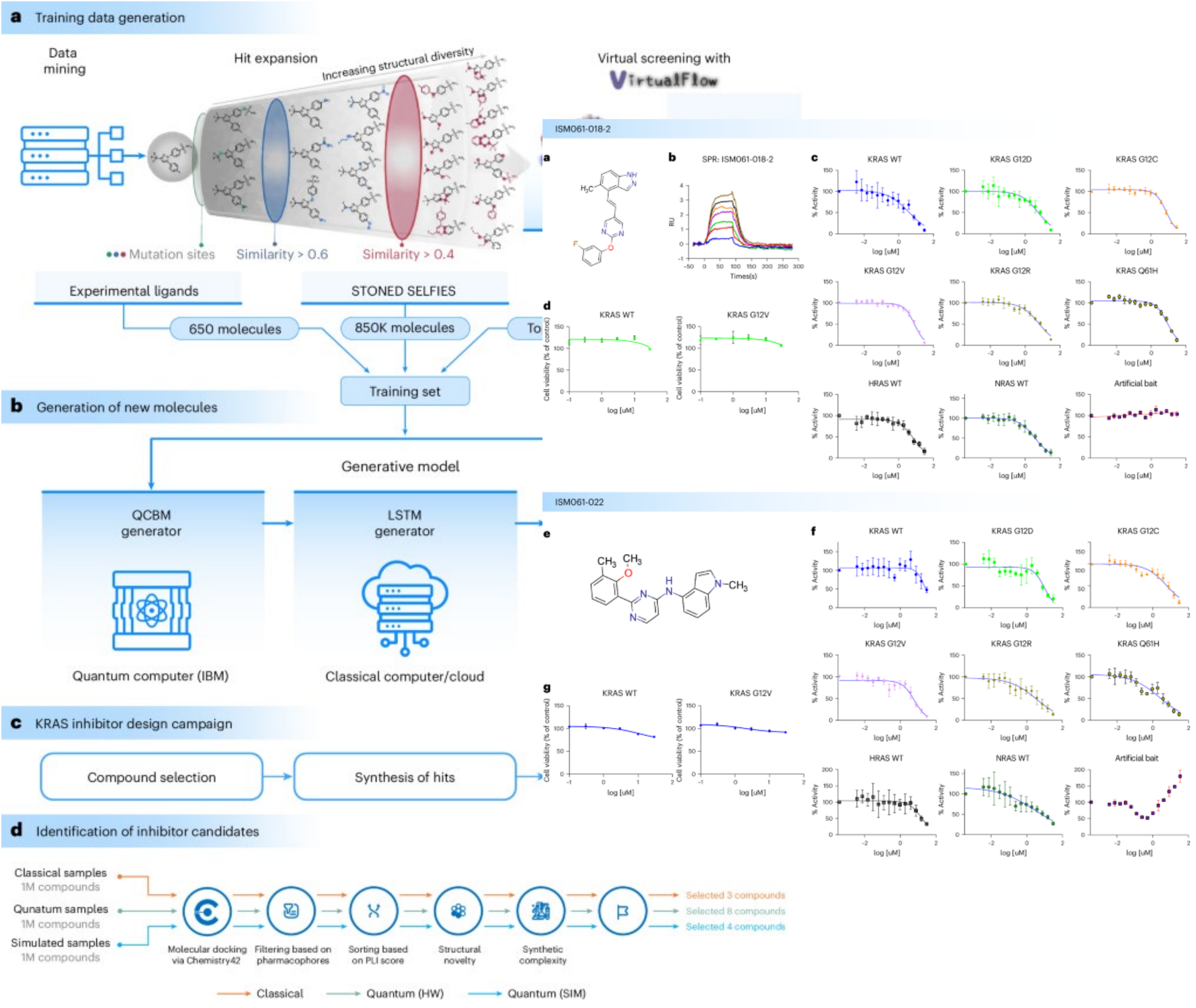
Quantum-computing-enhanced algorithm unveils potential KRAS inhibitors

Mohammad Ghazi Vakili, Christoph Gorgulla ✉, Jamie Snider, AkshatKumar Nigam ✉, Dmitry Bezrukov, Daniel Varoli, Alex Aliper, Daniil Polykovsky, Krishna M. Padmanabha Das, Huel Cox III, Anna Lyakisheva, Ardalan Hosseini Mansob, Zhong Yao, Lela Bitar, Danielle Tahoulas, Dora Čerina, Eugene Radchenko, Xiao Ding, Jinxin Liu, Fanye Meng, Feng Ren, Yudong Cao, Igor Stagljar ✉, Alán Aspuru-Guzik ✉ & Alex Zhavoronkov ✉

Nature Biotechnology (2025) | Cite this article

Abstract

We introduce a quantum–classical generative model for small-molecule design, specifically targeting KRAS inhibitors for cancer therapy. We apply the method to design, select and synthesize 15 proposed molecules that could notably engage with KRAS for cancer therapy, with two holding promise for future development as inhibitors. This work showcases the potential of quantum computing to generate experimentally validated hits that compare favorably against classical models.



PURDUE UNIVERSITY

Overview of Quantum Computing and applications in Chemical and Pharmaceutical Engineering

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May 8th, 2025

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