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Decomposition of problems: making problem easier for quantum computing

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April 1st, 2024

NSF Workshop on Post Quantum-AI

Indianapolis, Indiana

SECQUOIA

SYSTEMS ENGINEERING VIA CLASSICAL AND QUANTUM OPTIMIZATION FOR INDUSTRIAL APPLICATIONS

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Nonlinear discrete opt

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Q Federated Learning

Postdoc Carolina Tristán
Water Processes opt

PhD Albert Lee
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PhD Yirang Park
Quantum for Pharma

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Benchmarking Quantum

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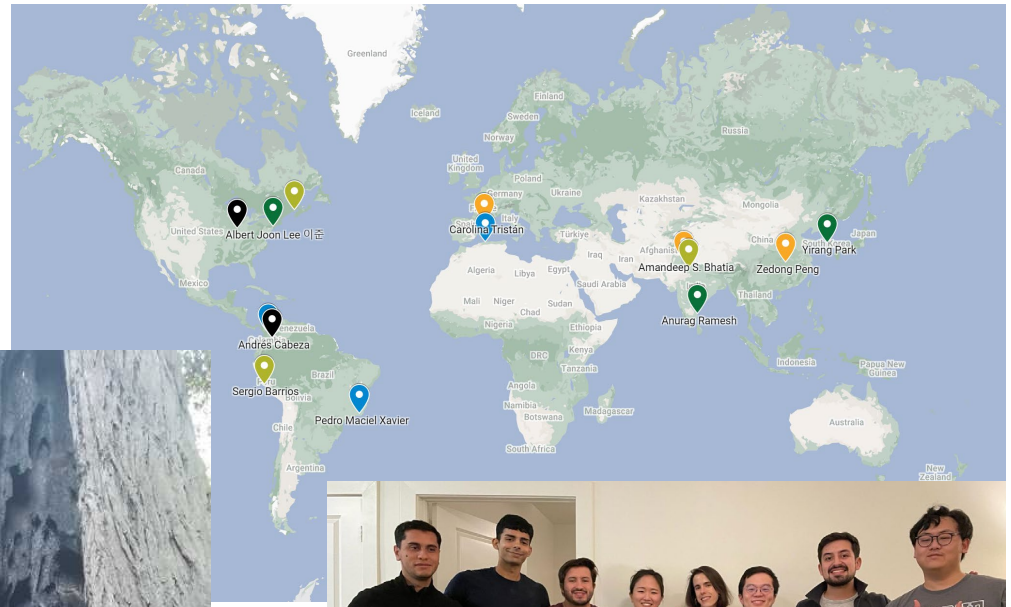
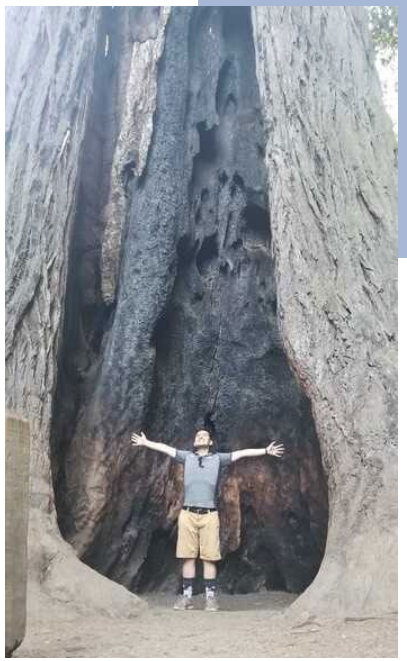
Process Intensification

Visitor Pedro Maciel Xavier
Quantum Computing

Visitor Juan Rodriguez
Process Scheduling





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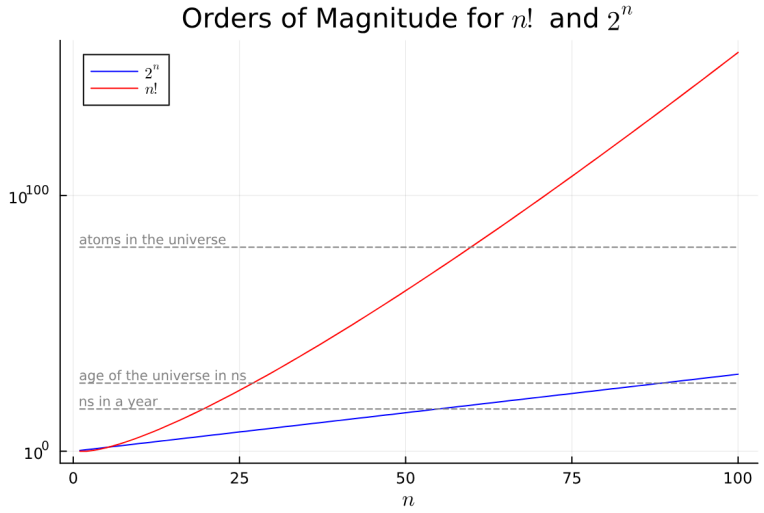
How can we tackle computationally Hard problems?

Enumerating solutions

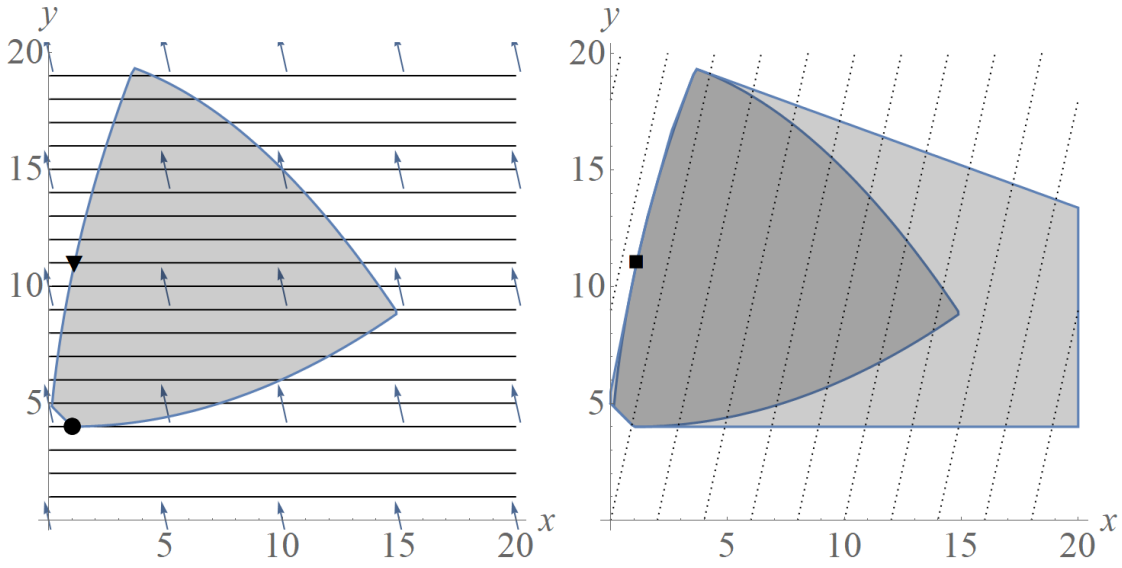
If we just look at **all the possible values**, check if they **satisfy the constraints** (being feasible) and **compare their objective**?

- Assuming only binary variables, the number of solutions grows as 2^n
- Many problems deal with permutations then number of solutions grows as $n!$



Decomposition methods

We can **split** these problems into **easily solvable** parts (**subproblems**) and **design algorithms** that put those parts together to find the complete solution to the problem.



Examples on tackling problems hard problem through decomposition – Quantum Optimization?

Formulations of many discrete optimization problems in Ising/QUBO

- Mappings of Karp's 21 NP-Complete problems to Ising and others

Some mappings are inefficient

"Reformulation" of discrete nonlinear optimization to Ising/QUBO

- Continuous variables – Discretize
- Integer variables – Binarize
- Nonlinear Equations – Quadratize
- Constraints – Penalize with ρ

Problem size growth

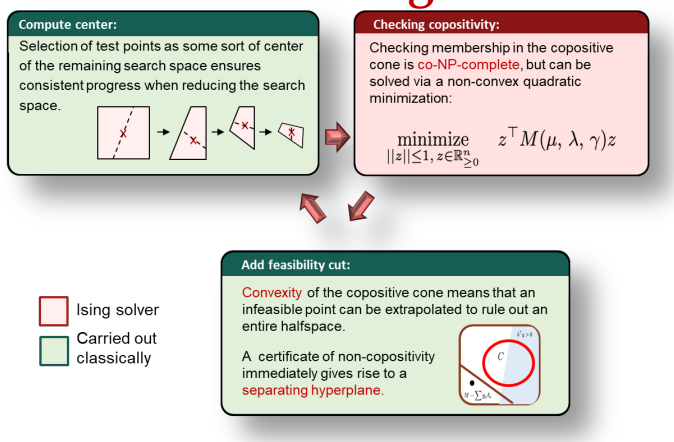
Extra variables and large coefficients

Extra variables

"Softening" of constraints

Decomposition Algorithms

- Alternating Direction Method of Multipliers (ADMM) [2]
- Test-set computation [3]
- Generator Enhanced Optimization [4]
- Copositive Programming-based cutting plane [5, Next slides]
- And many others!



1. Lucas, Andrew. "Ising formulations of many NP problems." Frontiers in physics 2 (2014): 5.
2. Gambella, Claudio, and Andrea Simonetto. "Multiblock ADMM heuristics for mixed-binary optimization on classical and quantum computers." IEEE Transactions on Quantum Engineering 1 (2020): 1-22.
3. Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing with application to non-linear integer programs." arXiv preprint arXiv:1902.04215 (2019).
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5. Brown et al. arXiv:2207.13630 (2022).

QUBO.jl: A Julia Ecosystem for Ising and QUBO optimization


Pedro Maciel Xavier


Pedro Ripper


Tiago Andrade


Joaquim Dias Garcia


Nelson Maculan

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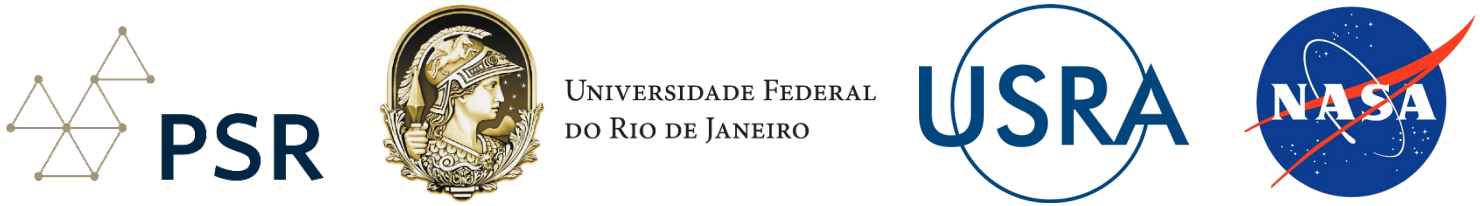

https://github.com/psrenergy/QUBO.jl

How do our Julia packages perform?

Outcome:
We provide the **fastest and most complete reformulator** of traditional optimization problems **to Ising/QUBO** as **open-source**

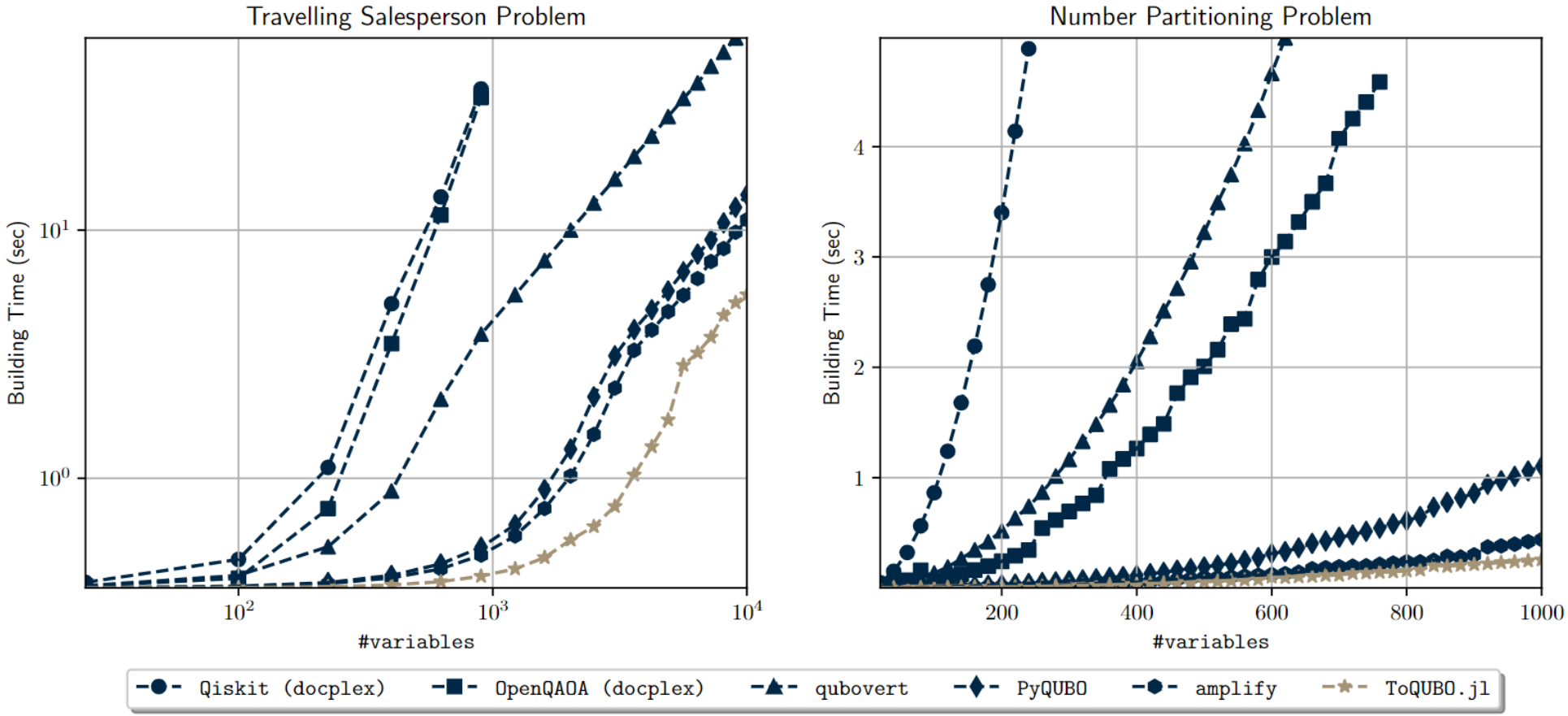

Figure 2 **Travelling Salesperson Problem in $\sqrt{\texttt{\#variables}}$ cities and NPP over $[\texttt{\#variables}] = \{1, \ldots, n\}$**

Copositive Optimization for mixed-binary quadratic optimization via Ising solvers

Robin Brown

Davide Venturelli

Marco Pavone

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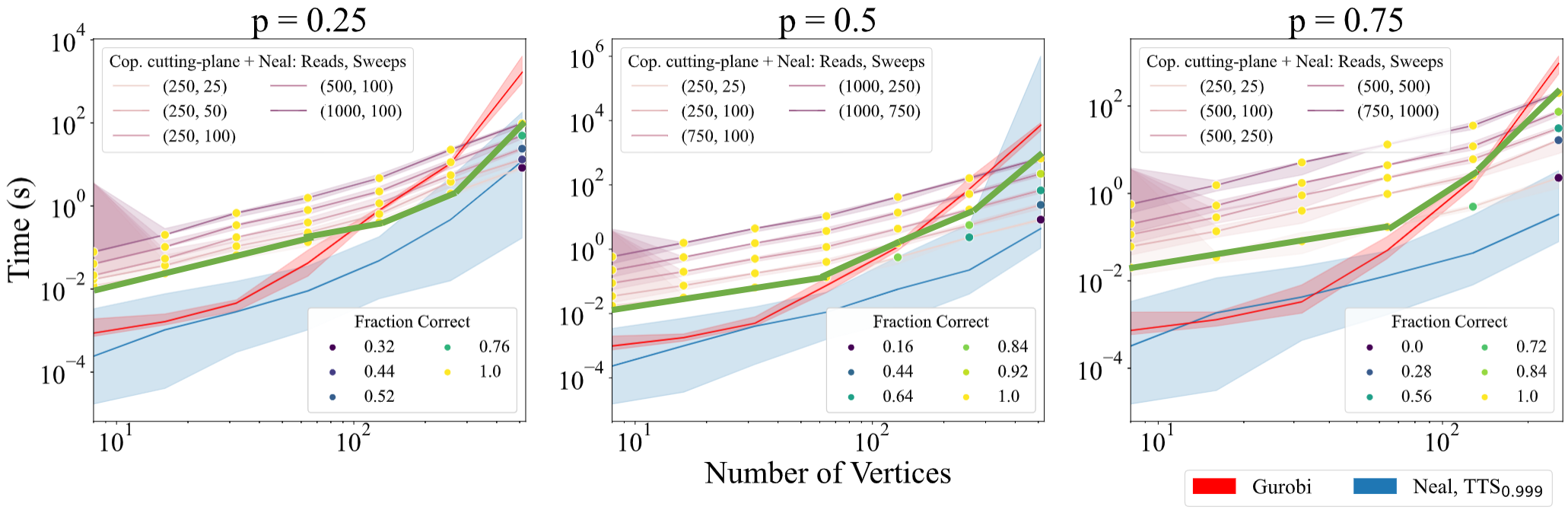
[3]Research Institute of Advanced Computer Science, USRA

arxiv.org/abs/2207.13630

How does this perform?

MAXCLIQUE comparison against MIP formulation and Ising heuristic



We

Solution time for the copositive cutting-plane algorithm with Simulated Annealing as the Ising solver, the solution time when solving a mixed-integer programming (MIP) formulation of maximum-clique directly with Gurobi, and the corresponding best penalty version of Simulated Annealing TTT to 99.9% confidence

QUANTUM COMPUTING IN CHEMICAL ENGINEERING

PERSPECTIVES ARTICLE AS INVITED CONTRIBUTION

AIChE JOURNAL
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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



NASA Carnegie Mellon University

Cornell University Founded A.D. 1865



ExxonMobil Research and Engineering

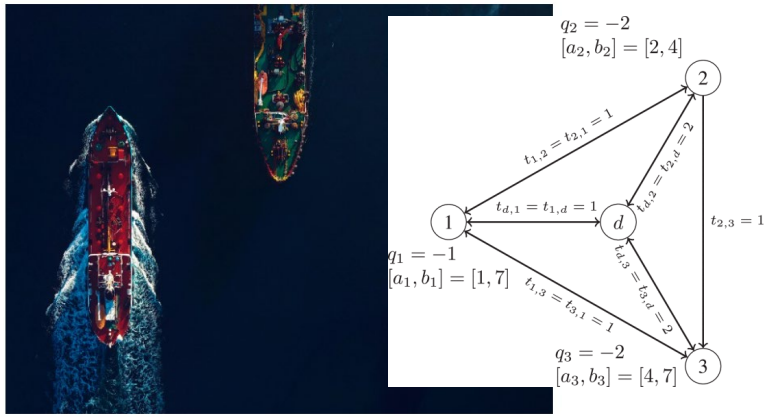
Current state of Quantum Computing leads us to identify **3 areas for ChemE with potential quantum advantage**

- Computational Chemistry
- Optimization
- Machine Learning

Although potential, there are still challenges to overcome

HYBRID QUANTUM CLASSICAL RESEARCH

Optimization [1]



(Image: Getty)

ExxonMobil & IBM Explore Quantum Algorithms to Solve Routing Formulations

https://ibm-research.medium.com/exxonmobil-ibm-scientists-explore-state-of-art-quantum-algorithms-to-solve-routing-formulations-e7ce39f8741c

Inside IBM Research 4 days ago · 5 min read

Computers and Chemical Engineering 184 (2024) 108627

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/cace

Utilizing modern computer architectures to solve mathematical optimization problems: A survey

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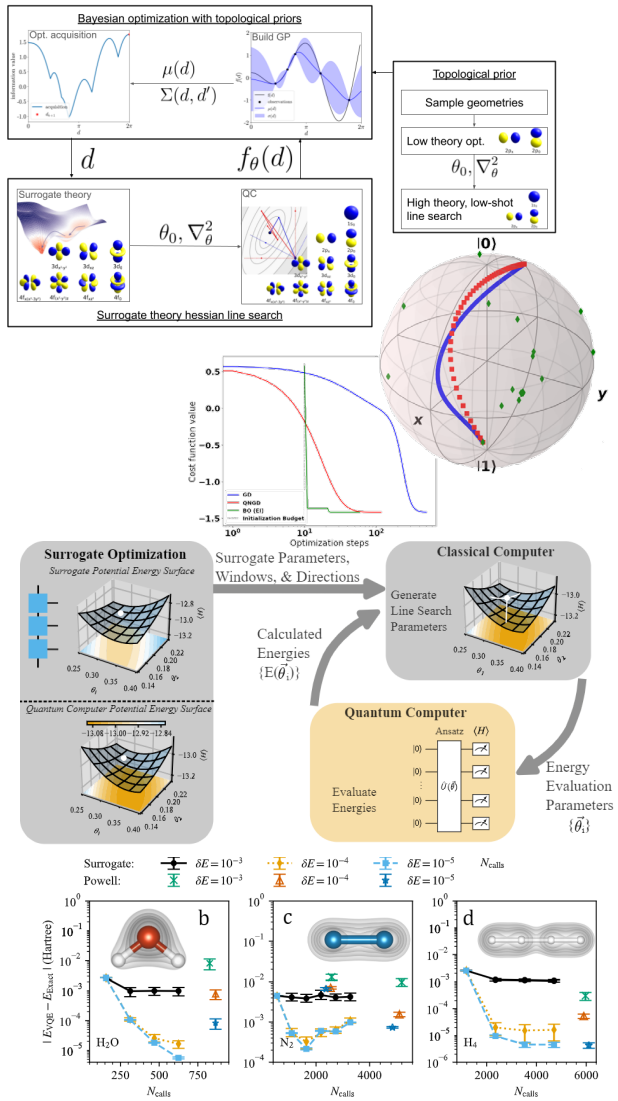
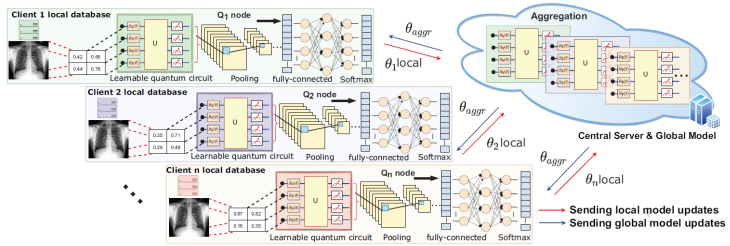
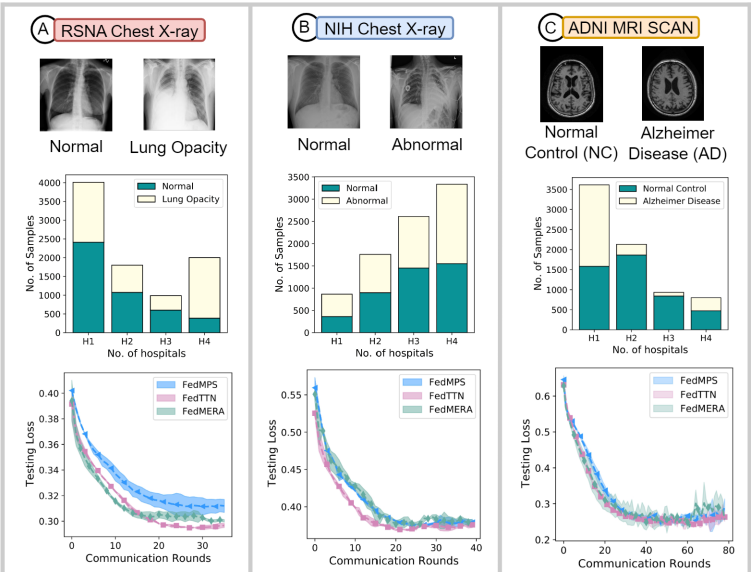
Computational Chemistry



Machine Learning





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