

# Quantum computing: a game-changing approach for drug development

## HMA/EMA Big Data Stakeholder Forum 2023

Albert H. Werner  
Associate Professor, Department for Mathematics  
QMATH & Quantum for Life Center

UNIVERSITY OF COPENHAGEN



# Quantum for Life Center

- Demonstrate the Viability of Quantum Computing to the Life Sciences



UNIVERSITY OF  
COPENHAGEN



Department of Mathematical Sciences  
Niels Bohr Institute  
Department of Computer Science

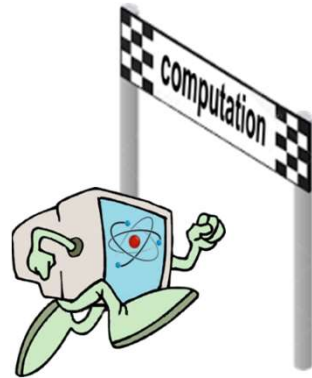
**ETH** zürich

Department of Chemistry and Applied Biosciences

# Overview

- Quantum Computing in Two Slides
- Quantum Simulation
- Applications for Drug Development

At the brink of becoming technology...

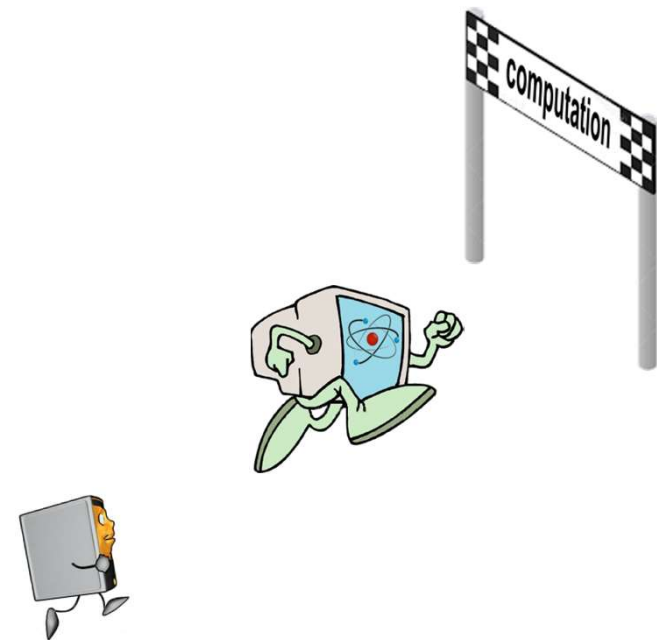


# What is a Quantum Computer?

- A device utilizing the laws of quantum mechanics for information processing
- Potential to solve certain problems faster than classical computers

## Quantum algorithms

- Shor's algorithm for factoring
- Sparse linear equation
- Semidefinite programs
- Big data/machine learning
- Quantum simulation

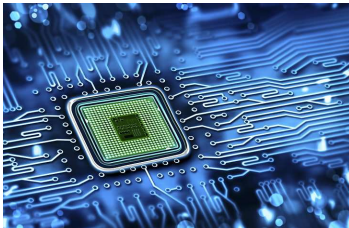


# Quantum vs. Classical Computer

0 ●

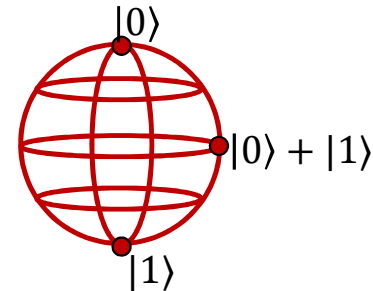
1 ●

**classical computer**

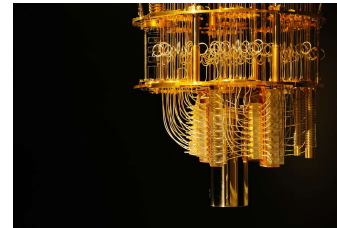


- bit: 0, 1
- dichotomic values

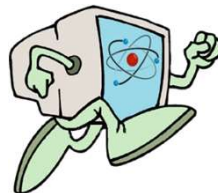
**More expressive!**



**quantum computer**



- qubit  $|0\rangle, |1\rangle$
- superposition principle
  - $|0\rangle + |1\rangle, |0\rangle - |1\rangle,$   
 $|0\rangle + i|1\rangle$



# Exponential growth in complexity

## single qubit

- superposition of 0 and 1

$$\alpha_0|0\rangle + \alpha_1|1\rangle$$

## two qubits

- superposition of 00, 01, 10, 11

$$\alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

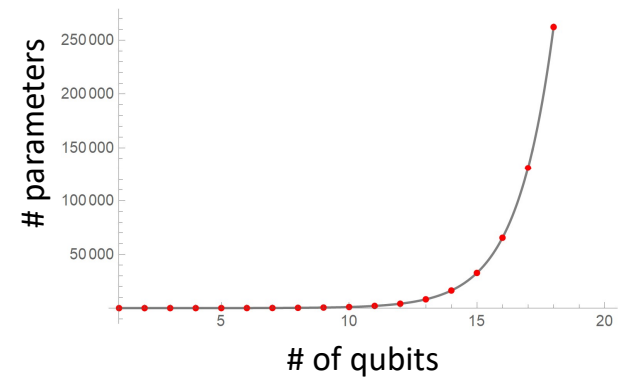
## three qubits

- superposition of 000, 001, 010, 011, 100, 101, 110, 111

$$\alpha_{000}|000\rangle + \alpha_{001}|001\rangle + \alpha_{010}|010\rangle + \alpha_{011}|011\rangle + \alpha_{100}|100\rangle + \alpha_{101}|101\rangle + \alpha_{110}|110\rangle + \alpha_{111}|111\rangle$$

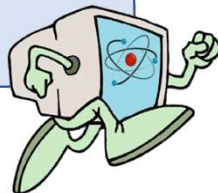
## n qubits

- superposition of  $2^n$  classical states

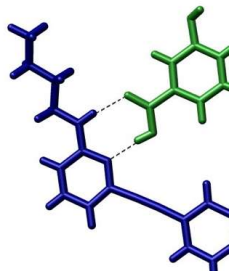


**exponential growth of free parameters**  
**exponential memory requirements**

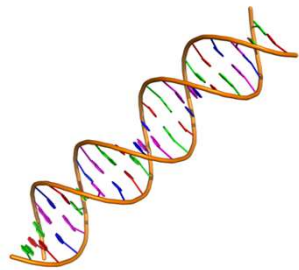
**Hard to simulate on classical computer!**  
**Potential for quantum speedups!**



# Quantum Simulation



docking of molecule



DNA molecule

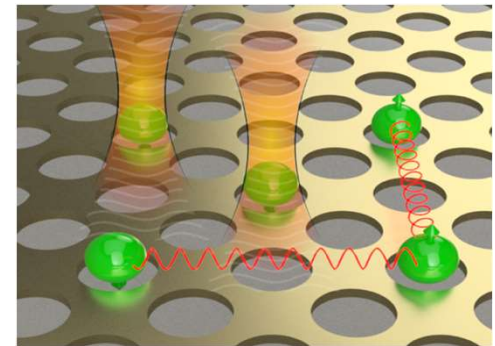
$$i\hbar \frac{\partial \Psi(t)}{\partial t} = H \Psi(t)$$

Hamiltonian

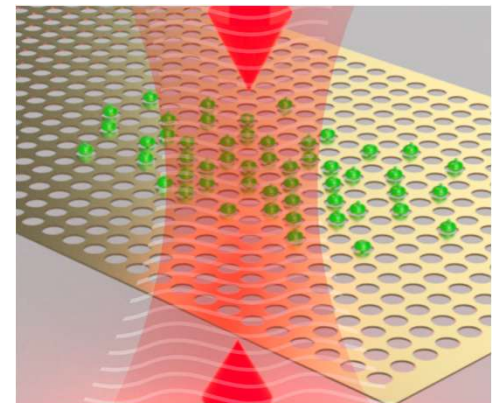
Schrödinger equation



Richard Feynman

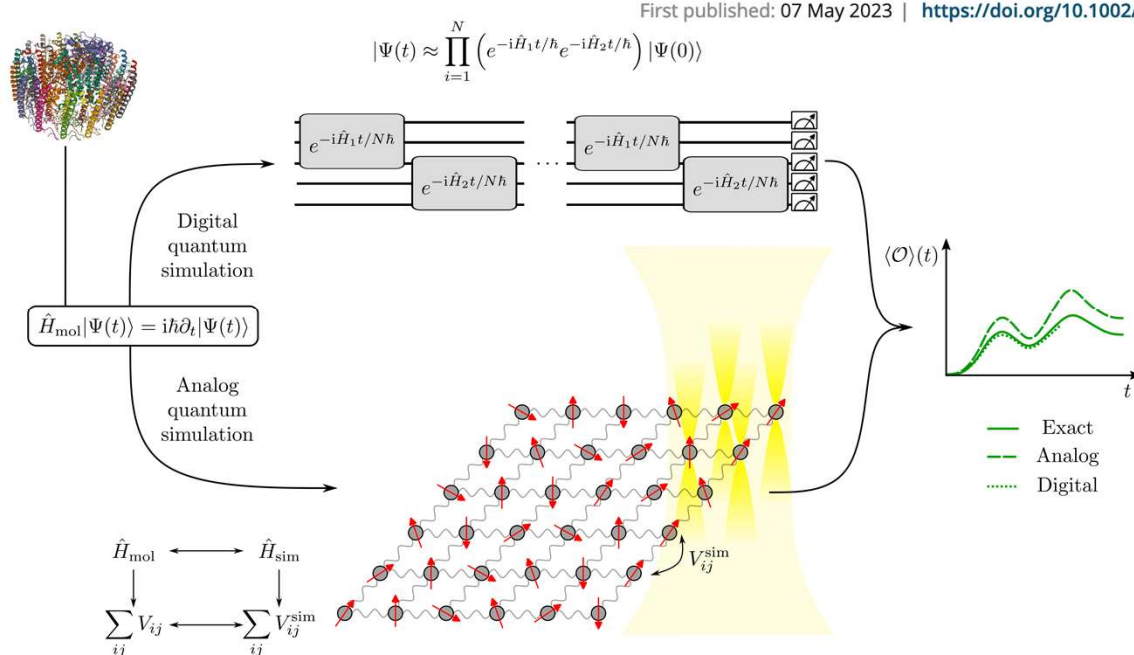
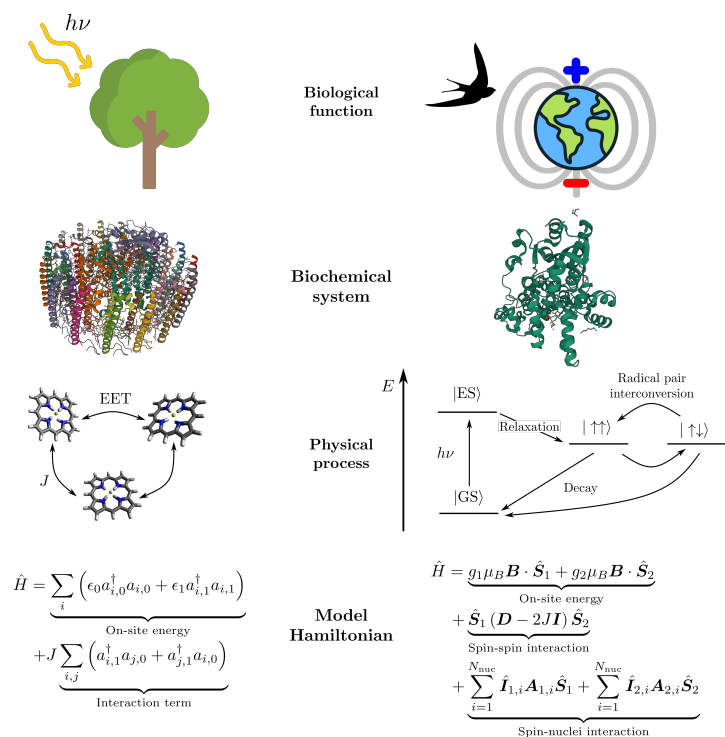


quantum simulation

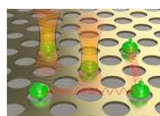
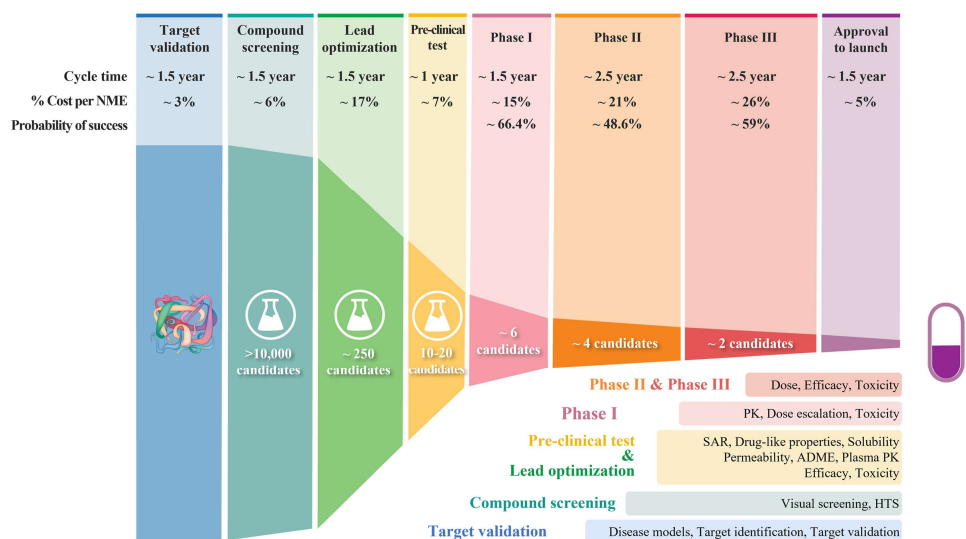


quantum machine learning

# Quantum Algorithms



# Quantum Computing for Drug Discovery



quantum simulation



Informatics (orange)  
**Quantum computing's potential for drug discovery: Early stage industry dynamics**

## Potential of quantum computing for drug discovery

Publisher: IBM [Cite This](#) [PDF](#)

Y. Cao ; J. Romero ; A. Aspuru-Guzik [All Authors](#)

**JCTC**  
 Journal of Chemical Theory and Computation

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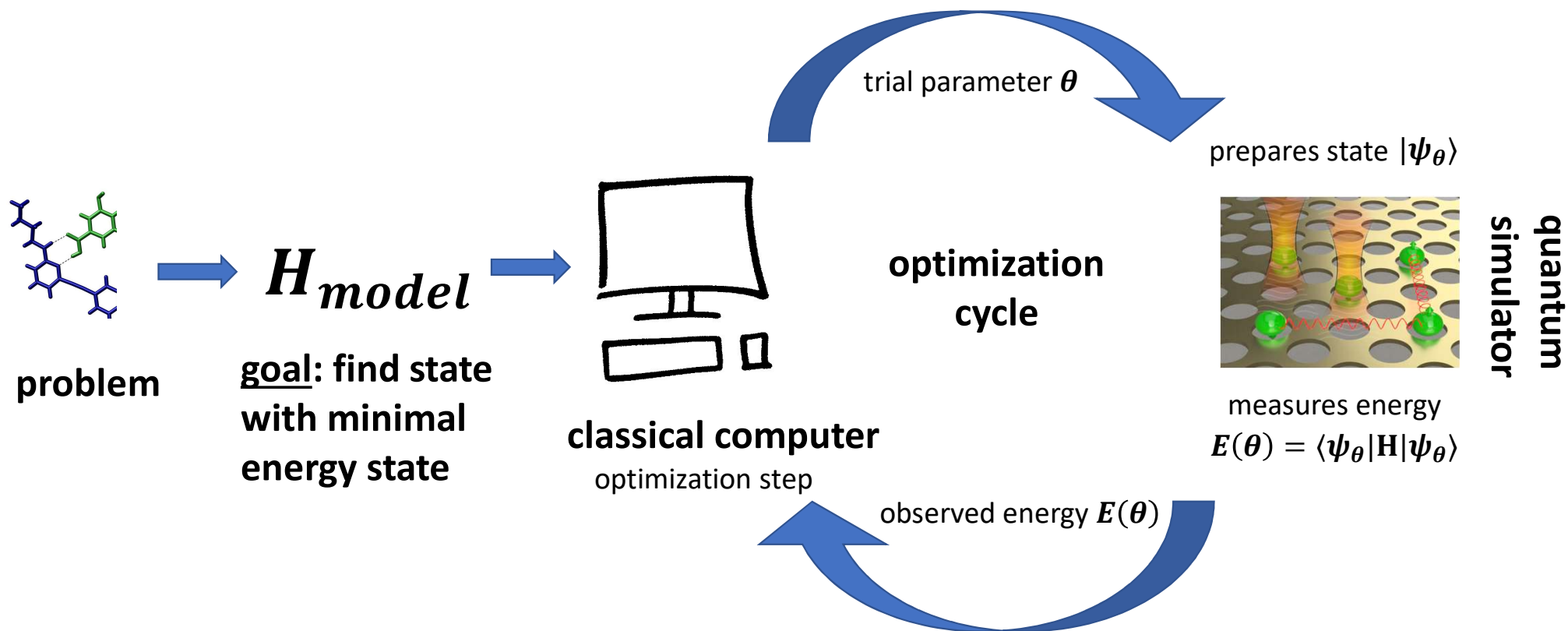


Perspective

## Perspective on the Current State-of-the-Art of Quantum Computing for Drug Discovery Applications

Nick S. Blunt,<sup>§</sup> Joan Camps,<sup>§</sup> Ophelia Crawford,<sup>§</sup> Róbert Izsák,<sup>§</sup> Sebastian Leontica,<sup>§</sup> Arjun Mirani,<sup>§</sup> Alexandra E. Moylett,<sup>§</sup> Sam A. Scivier,<sup>§</sup> Christoph Sünderhauf,<sup>§</sup> Patrick Schopf, Jacob M. Taylor, and Nicole Holzmann\*

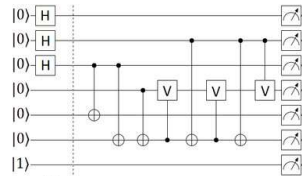
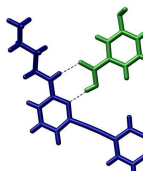
# Variational Quantum Eigensolver



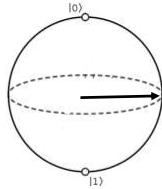
# An Interdisciplinary Challenge



problem identification



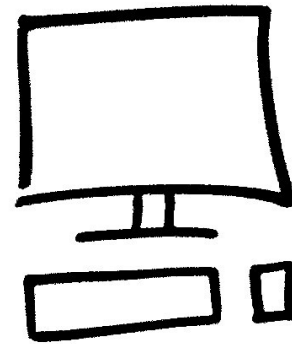
quantum algorithms



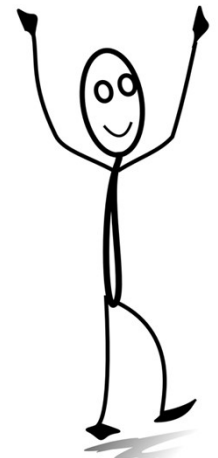
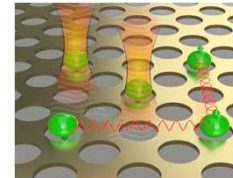
necessary



powers



experimental quantum simulator



proof-of-principle demonstration

