Quantum Control in the Era of Quantum Computing

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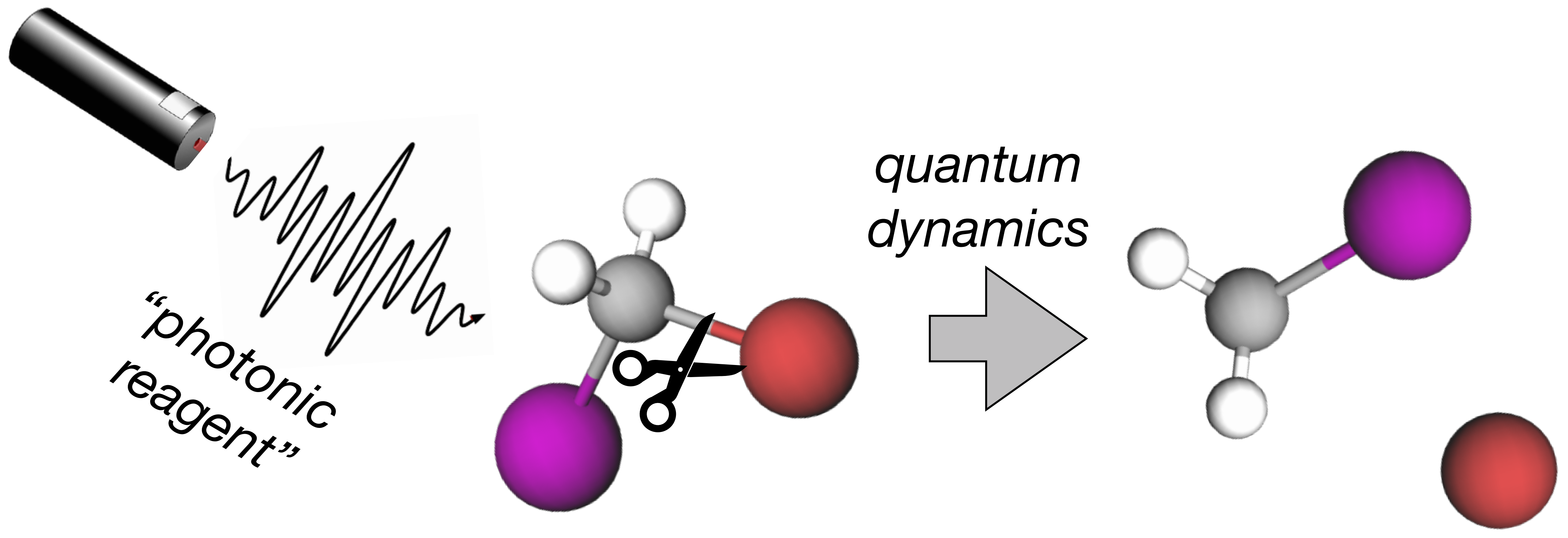
Controlling chemistry with light

Lasers can create tailored light to control chemical transformations that would not otherwise be possible

- selective bond-breaking
- molecular rearrangement
- molecular orientation
- isotope selective processes
- charge and energy transfer
- etc…

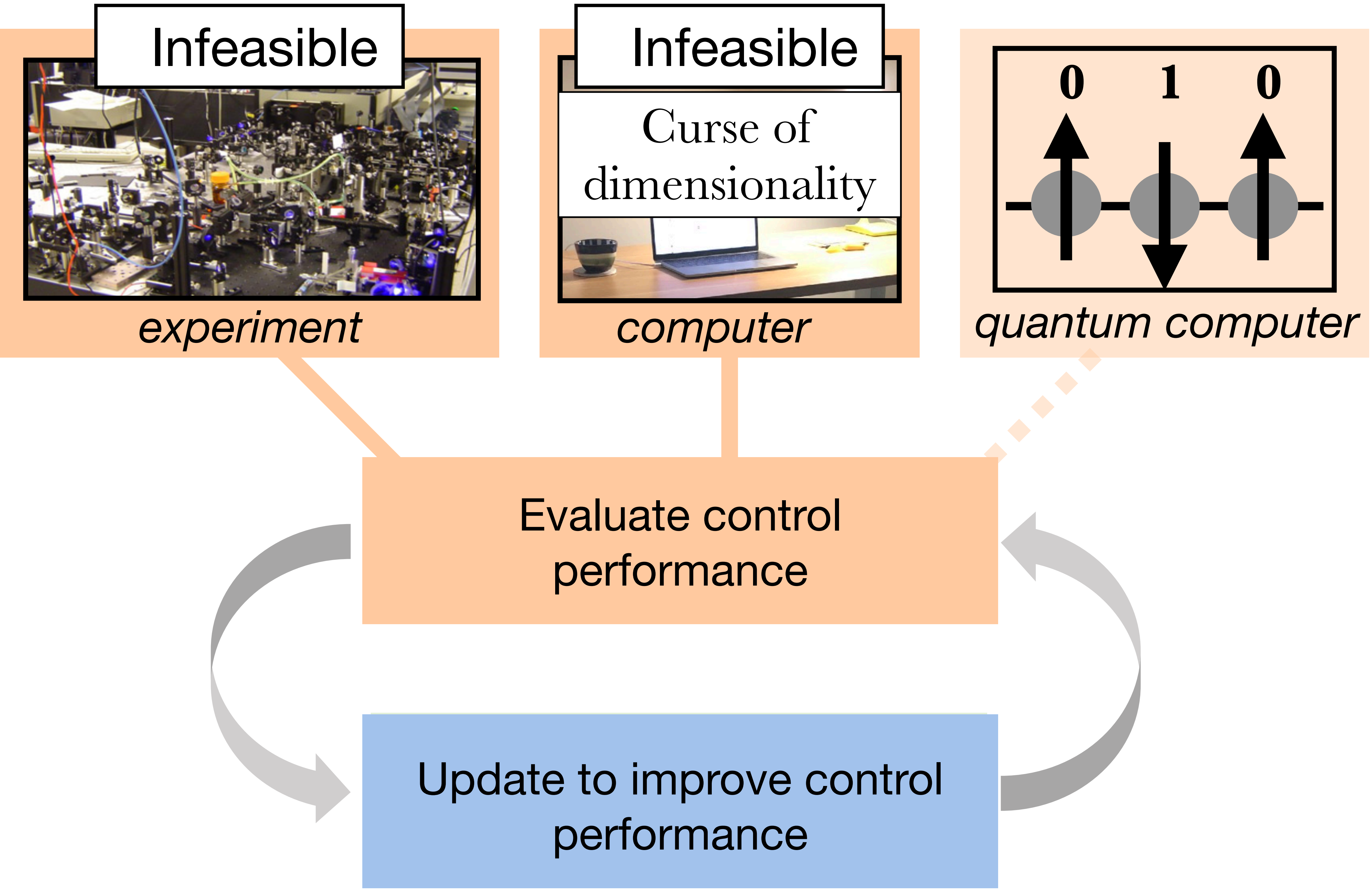


Designing photonic reagents is hard - so far only proof-of-principle demonstrations in experiments

Progress is limited by the computational difficulty of simulation support

This Talk:
Quantum computing for enabling chemistry with photonic reagents

Quantum optimal control

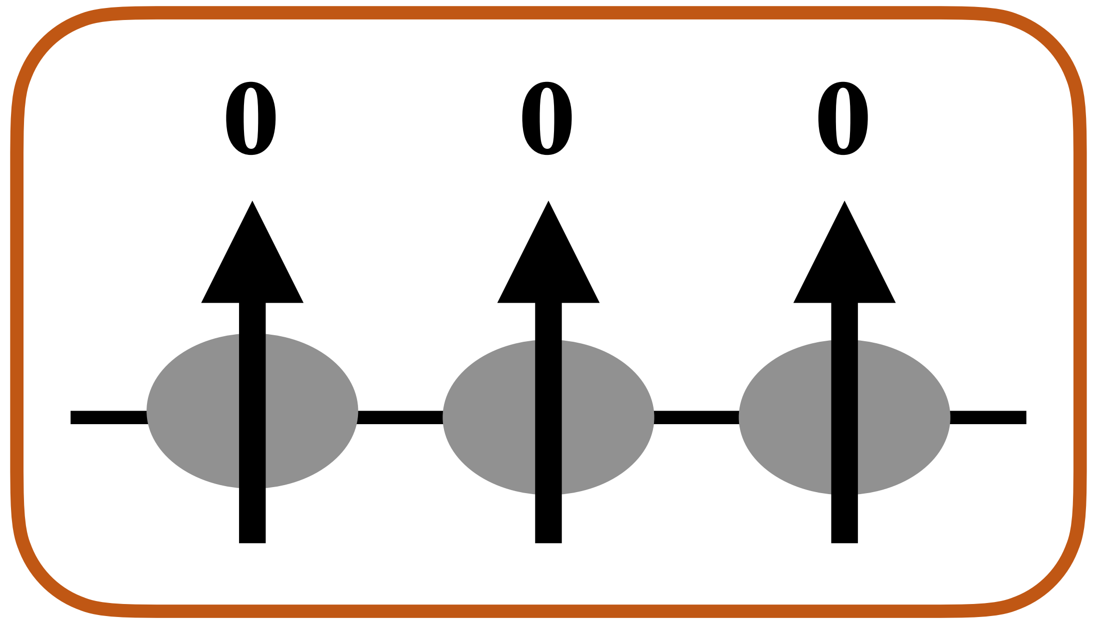


Quantum computing

Classical computing: store information in bits which can be 0 or 1, do logical operations on these bits

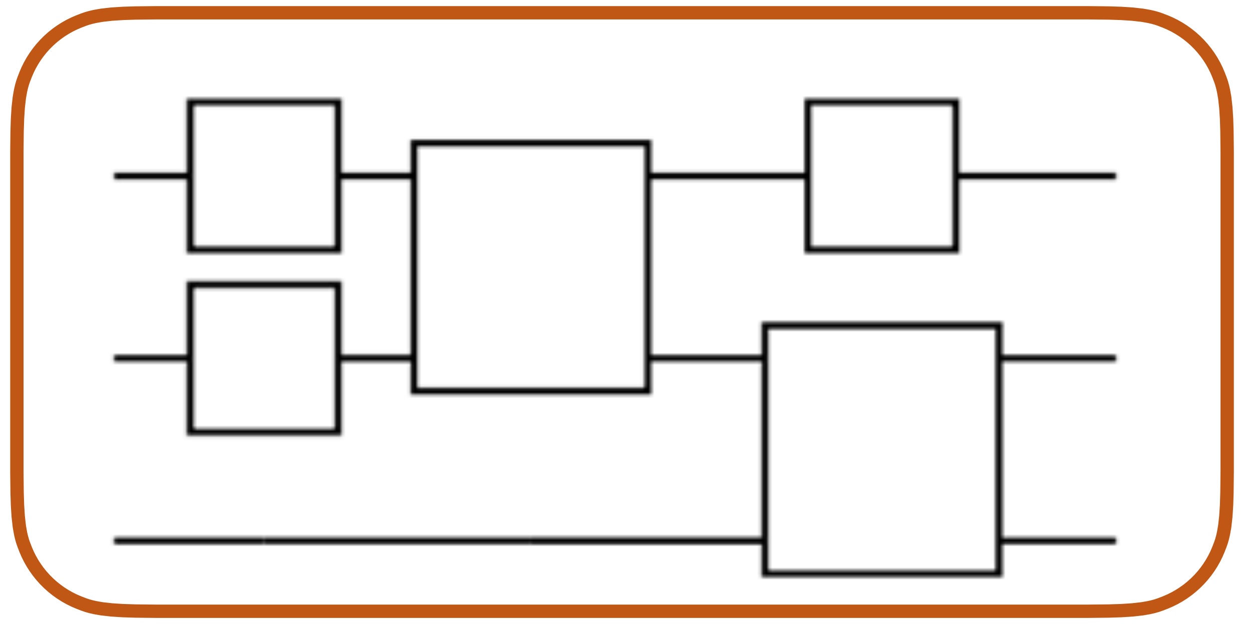
Quantum computing: store bits in the state of a quantum object - “qubits”

Initialization



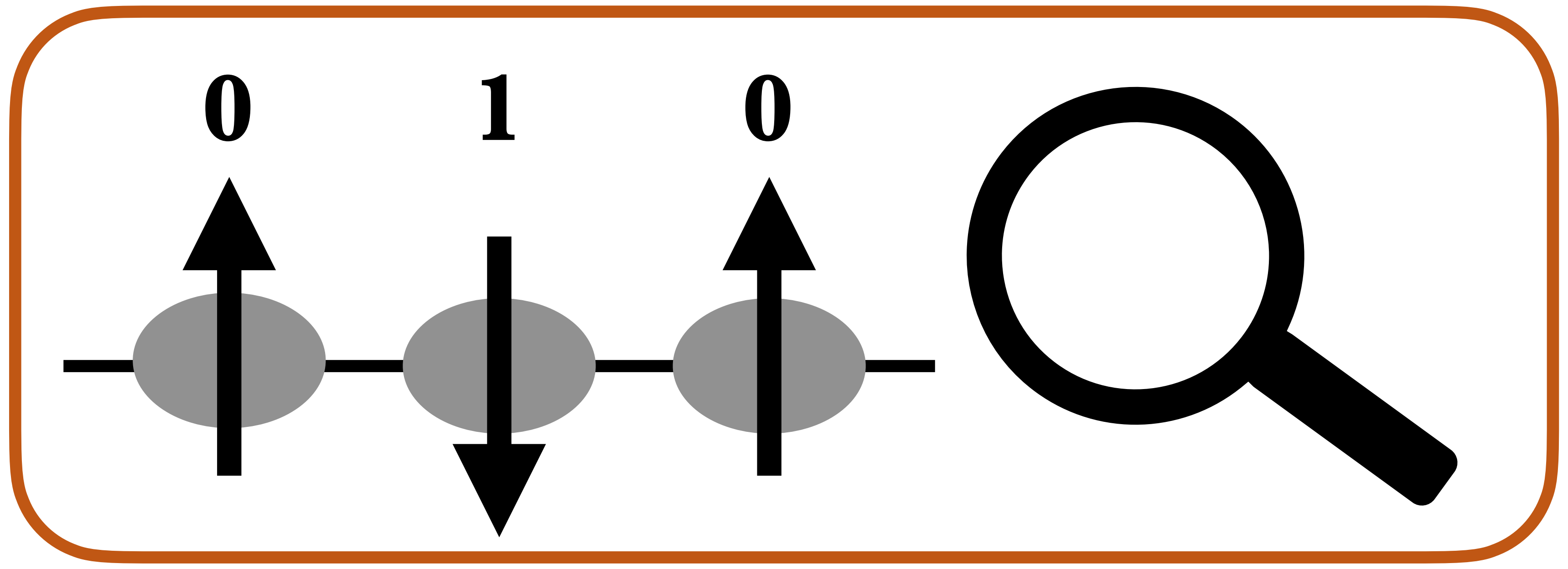
Prepare qubits in a specified initial state

Computation



Apply a sequence of gates to the qubits in order to perform computation

Readout



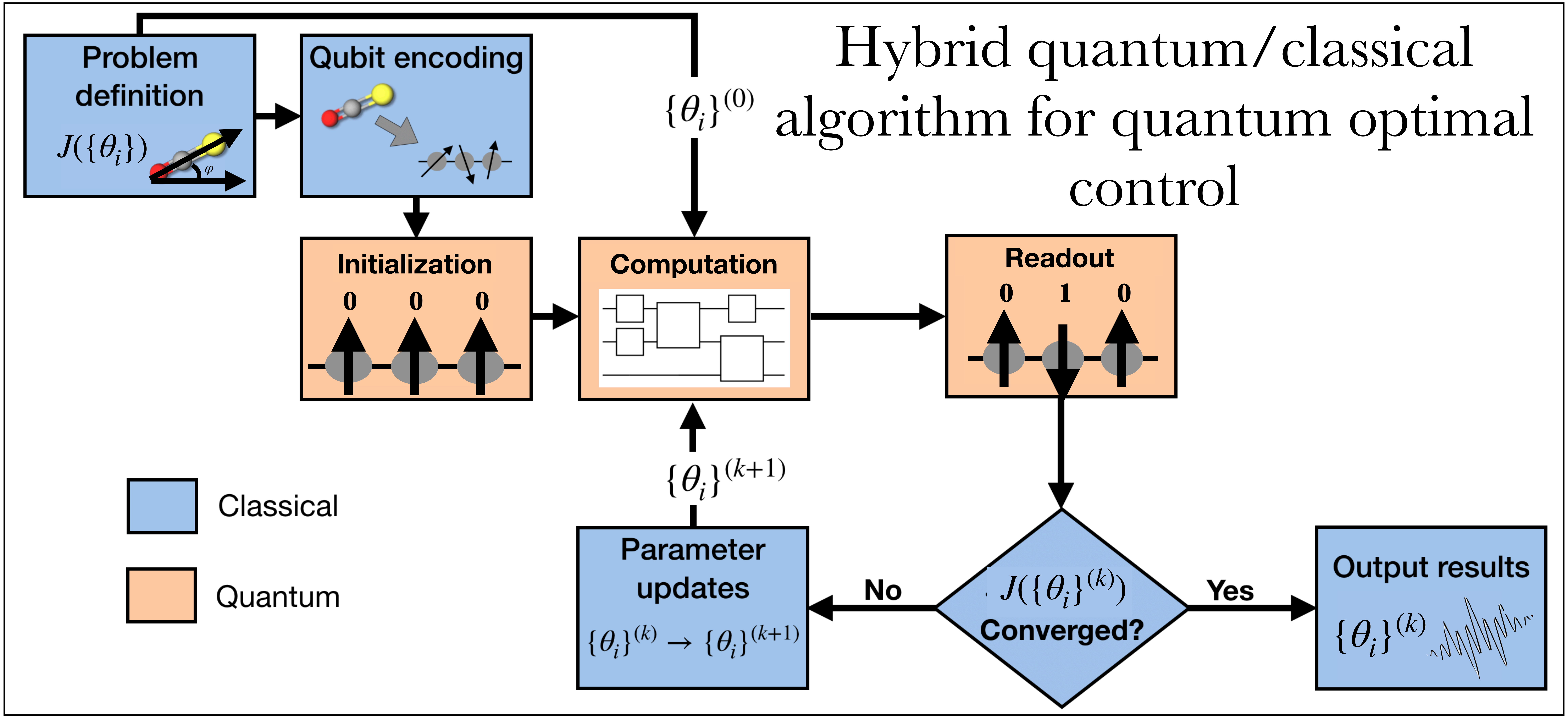
Measure the qubits to read out the results of the computation

Landmark papers from 1990’s showing quantum speedup for factoring, quantum simulation, unstructured search

Worldwide engagement in developing these quantum computing capabilities

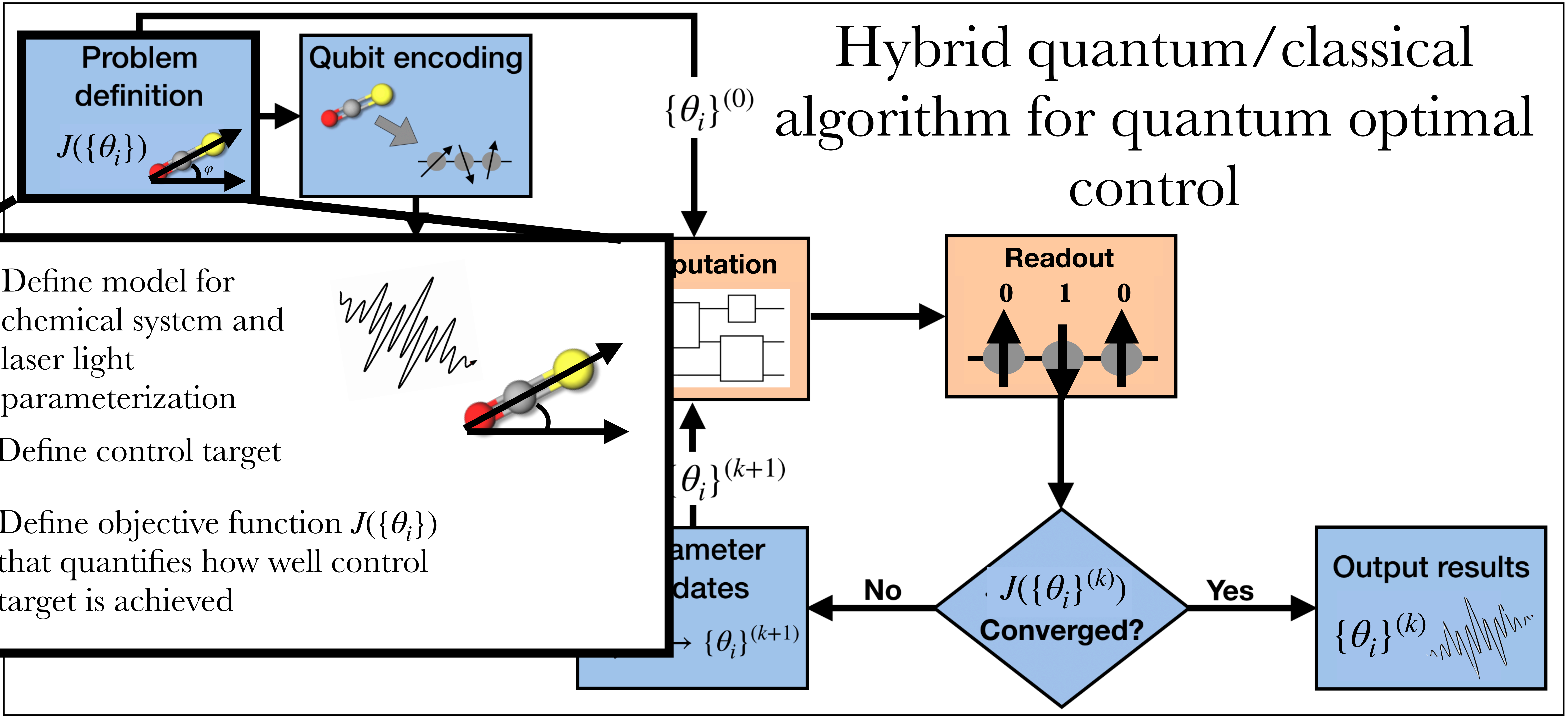
Today:
Intense interest in hybrid quantum-classical algorithms

Hybrid quantum/classical algorithm for quantum optimal control



AB Magann, MD Grace, HA Rabitz, M Sarovar, Phys. Rev. Research **3**, 023165 (2021)

Hybrid quantum/classical algorithm for quantum optimal control



- Define model for chemical system and laser light parameterization
- Define control target
- Define objective function $J(\{\theta_i\})$ that quantifies how well control target is achieved

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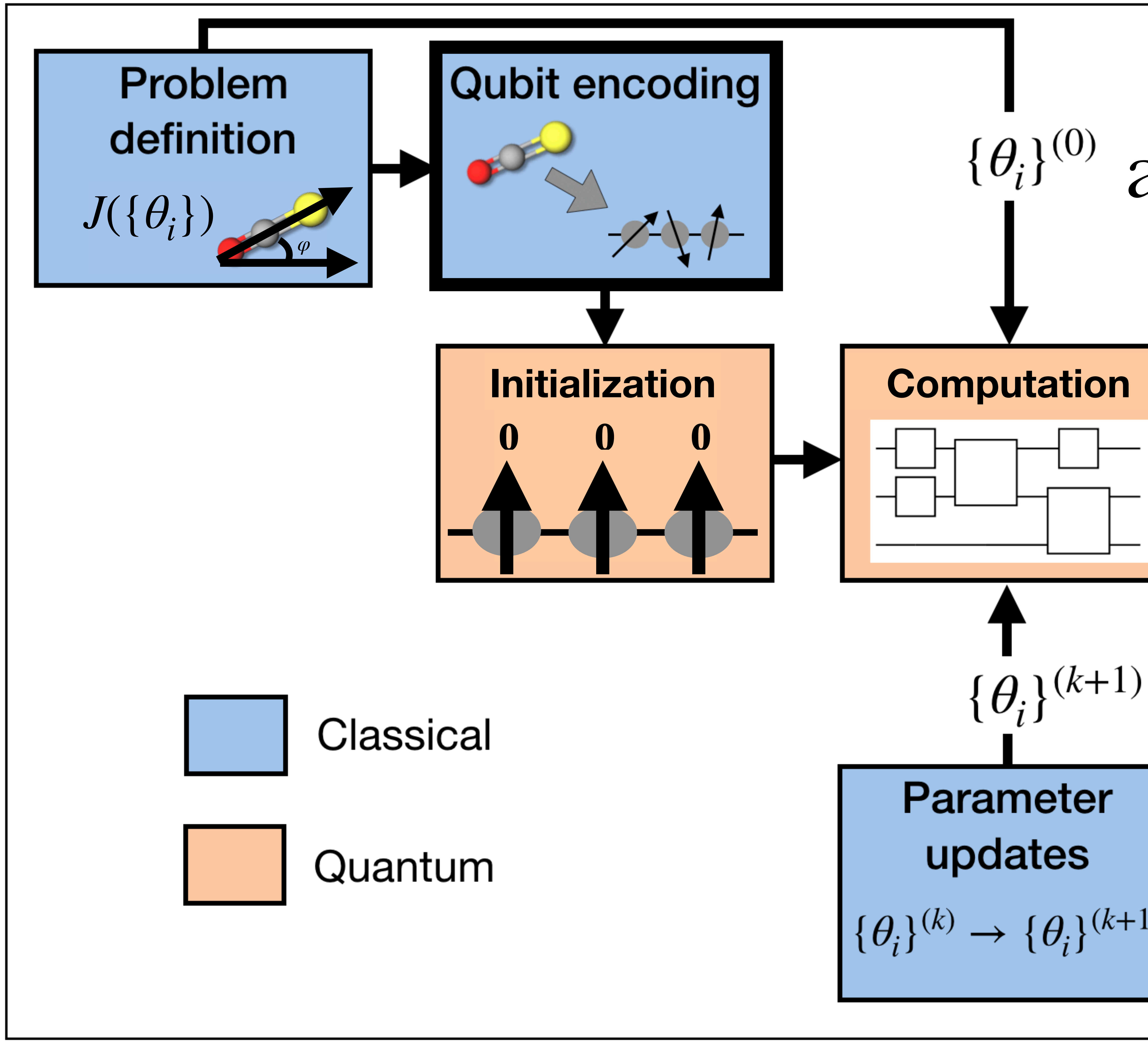

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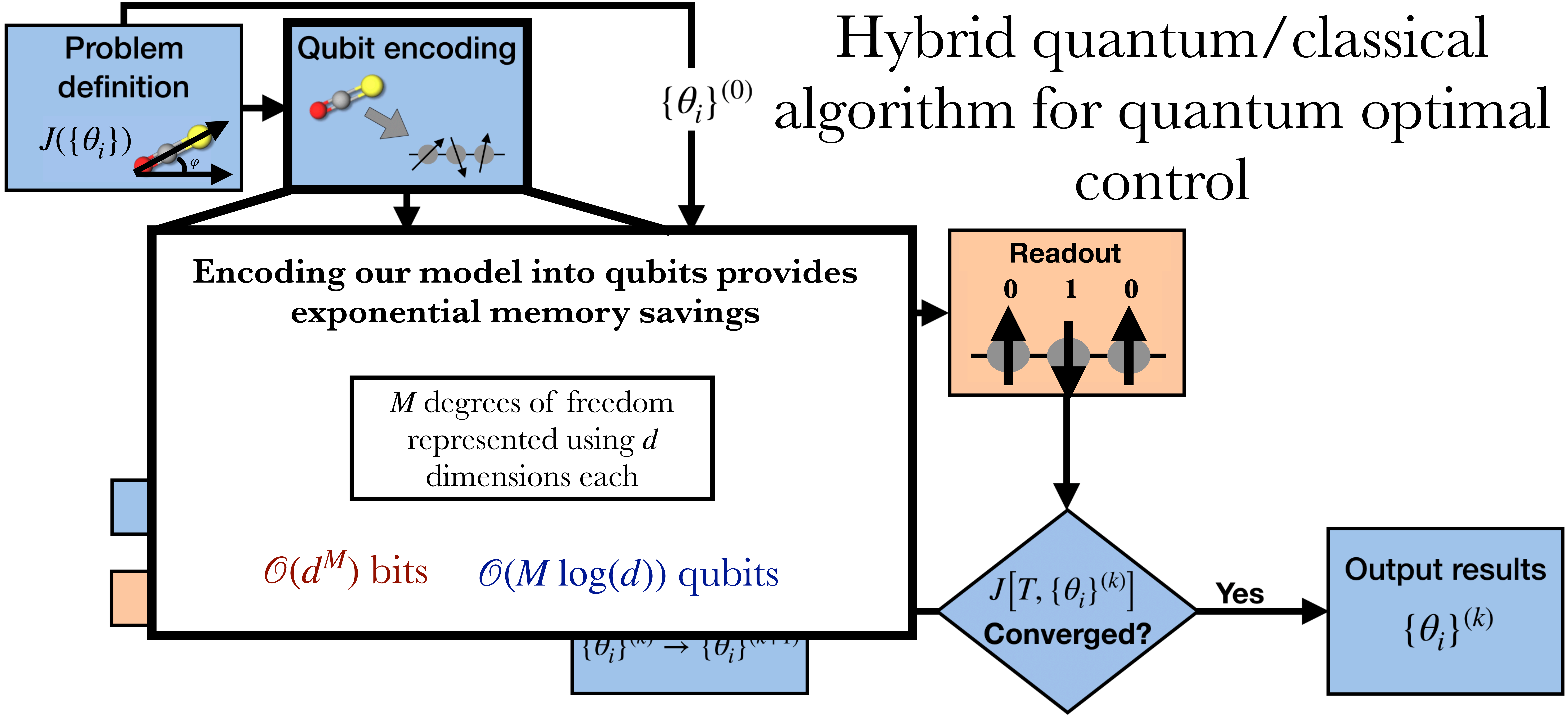

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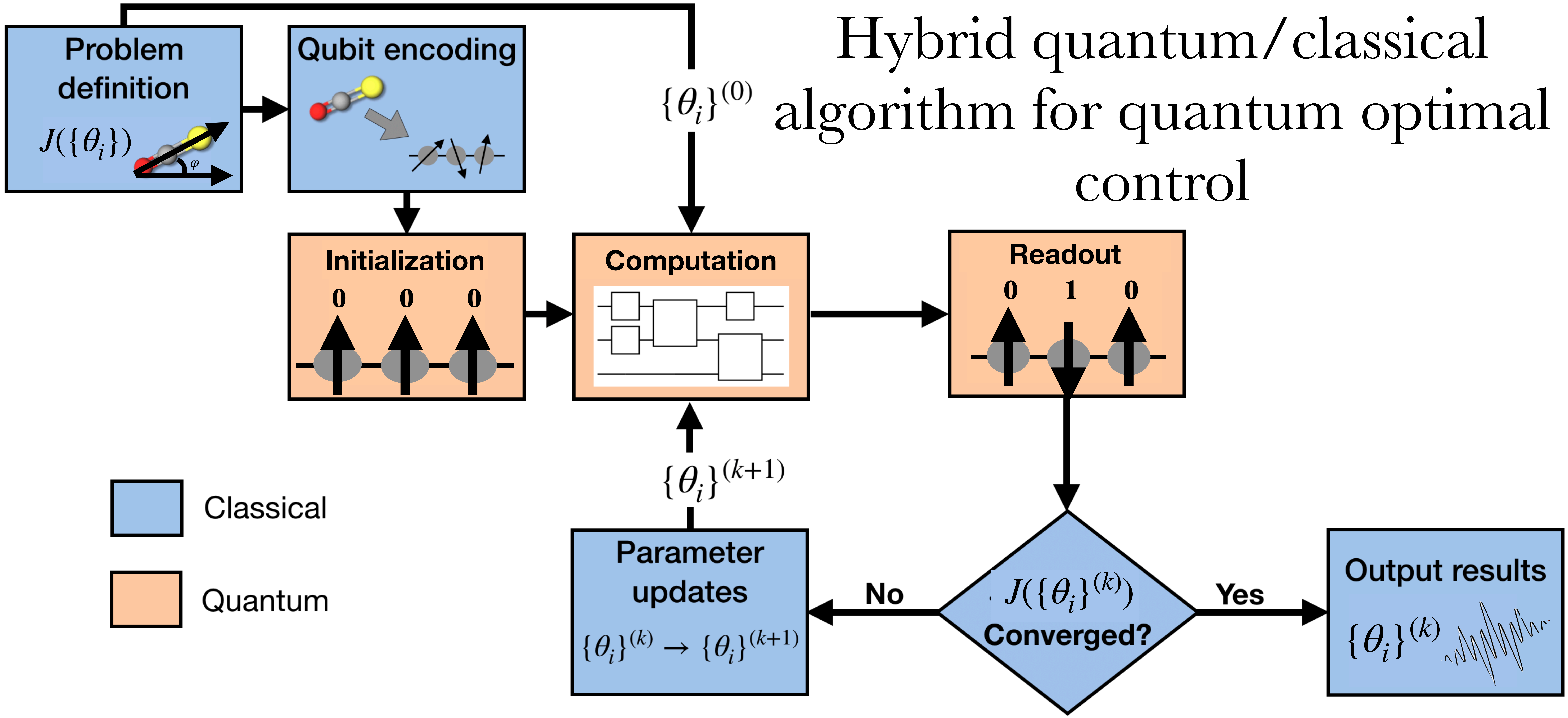

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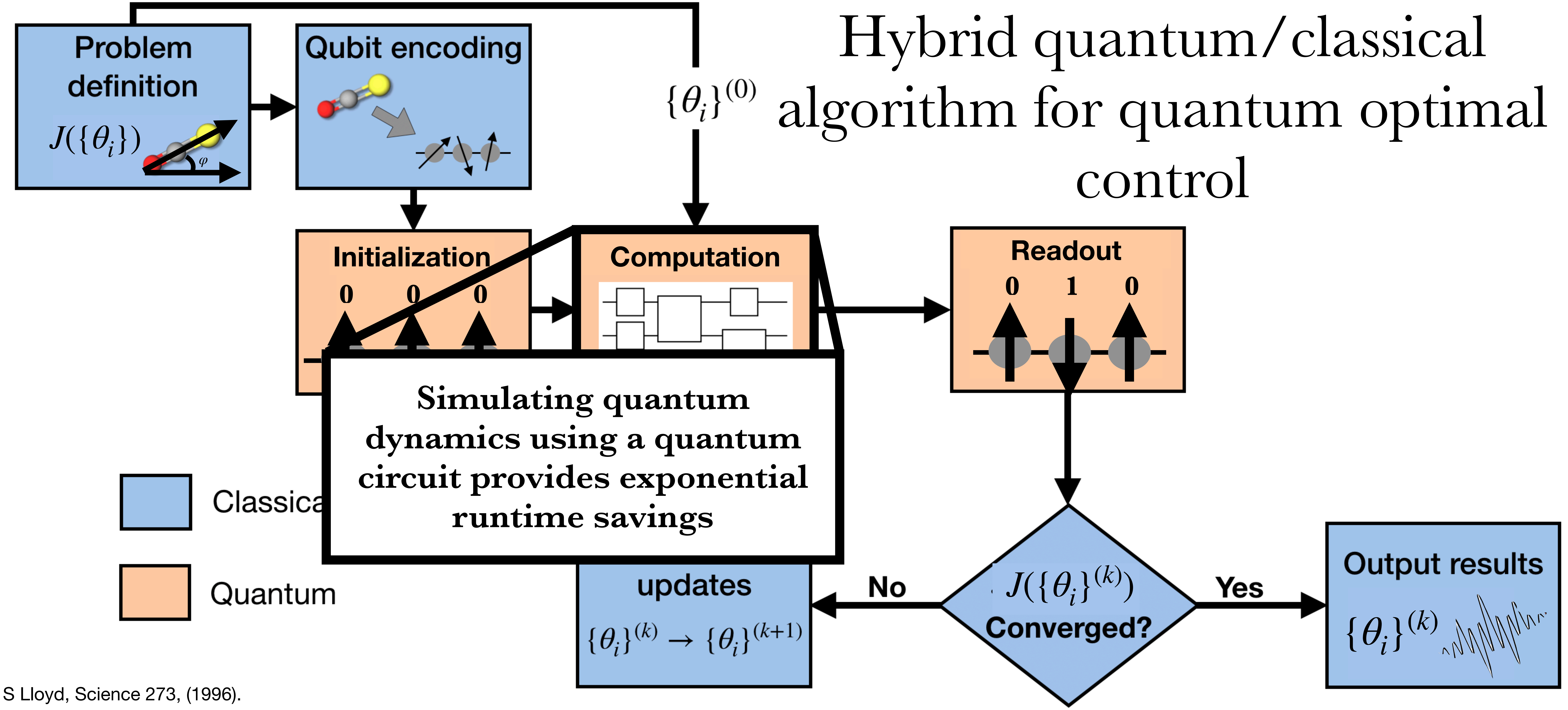

S Lloyd, Science 273, (1996).

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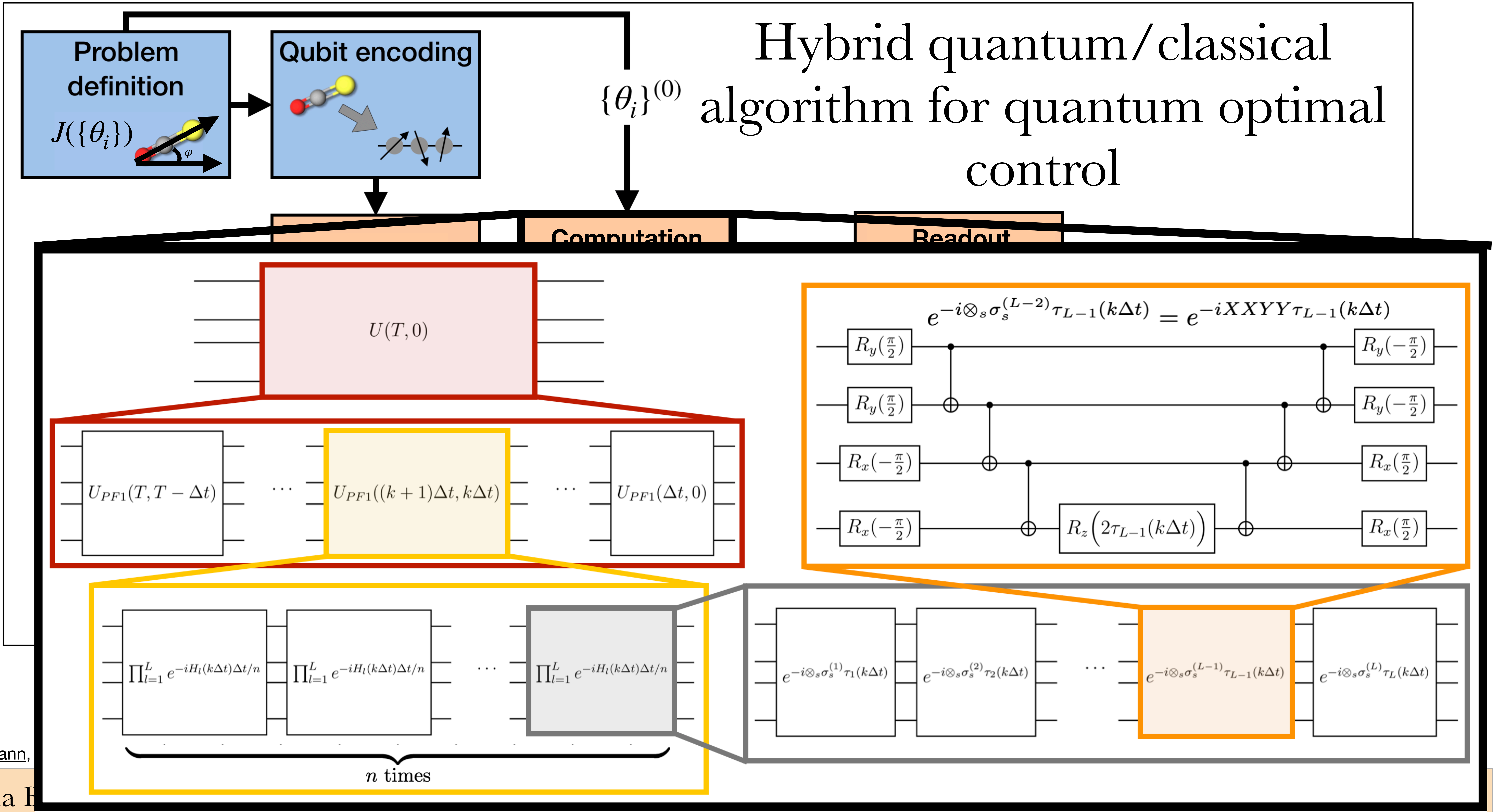

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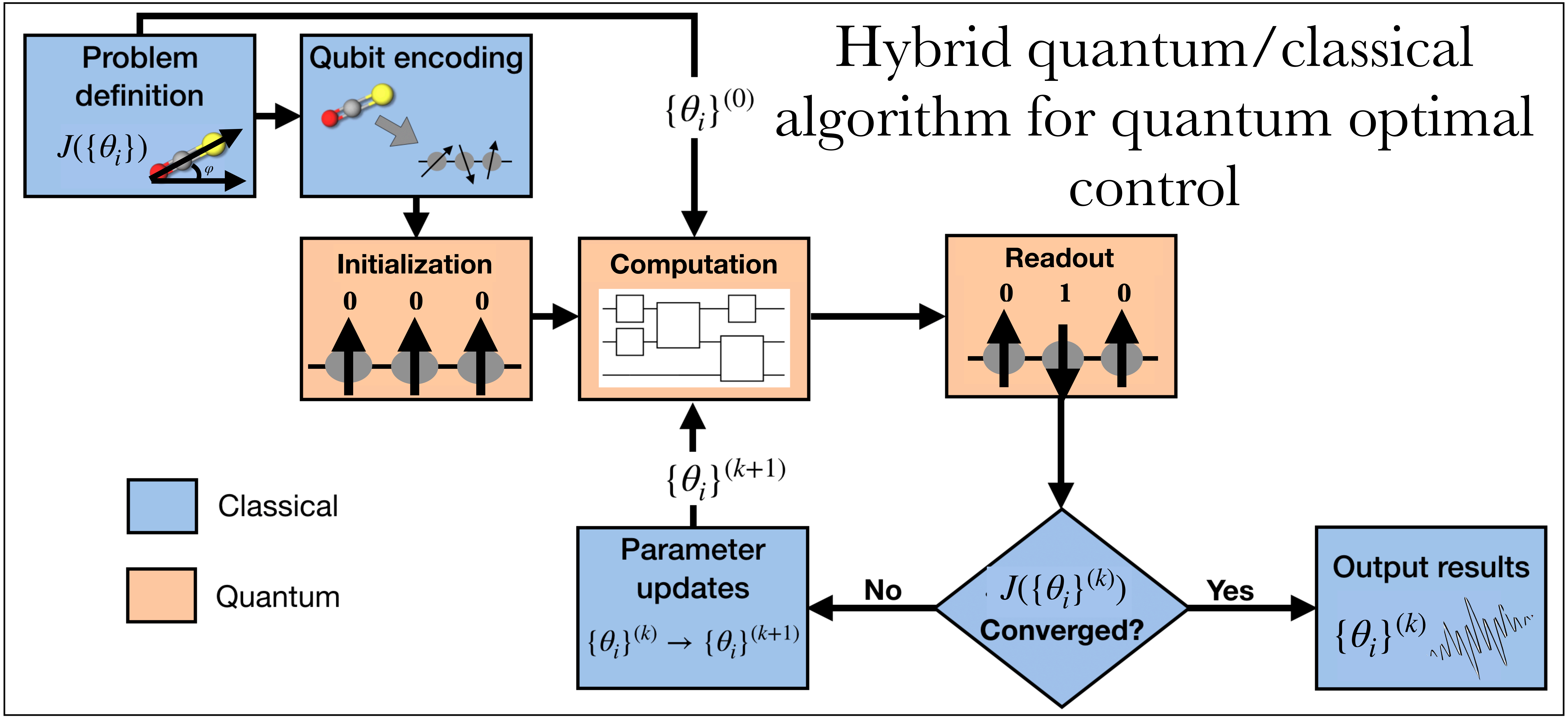

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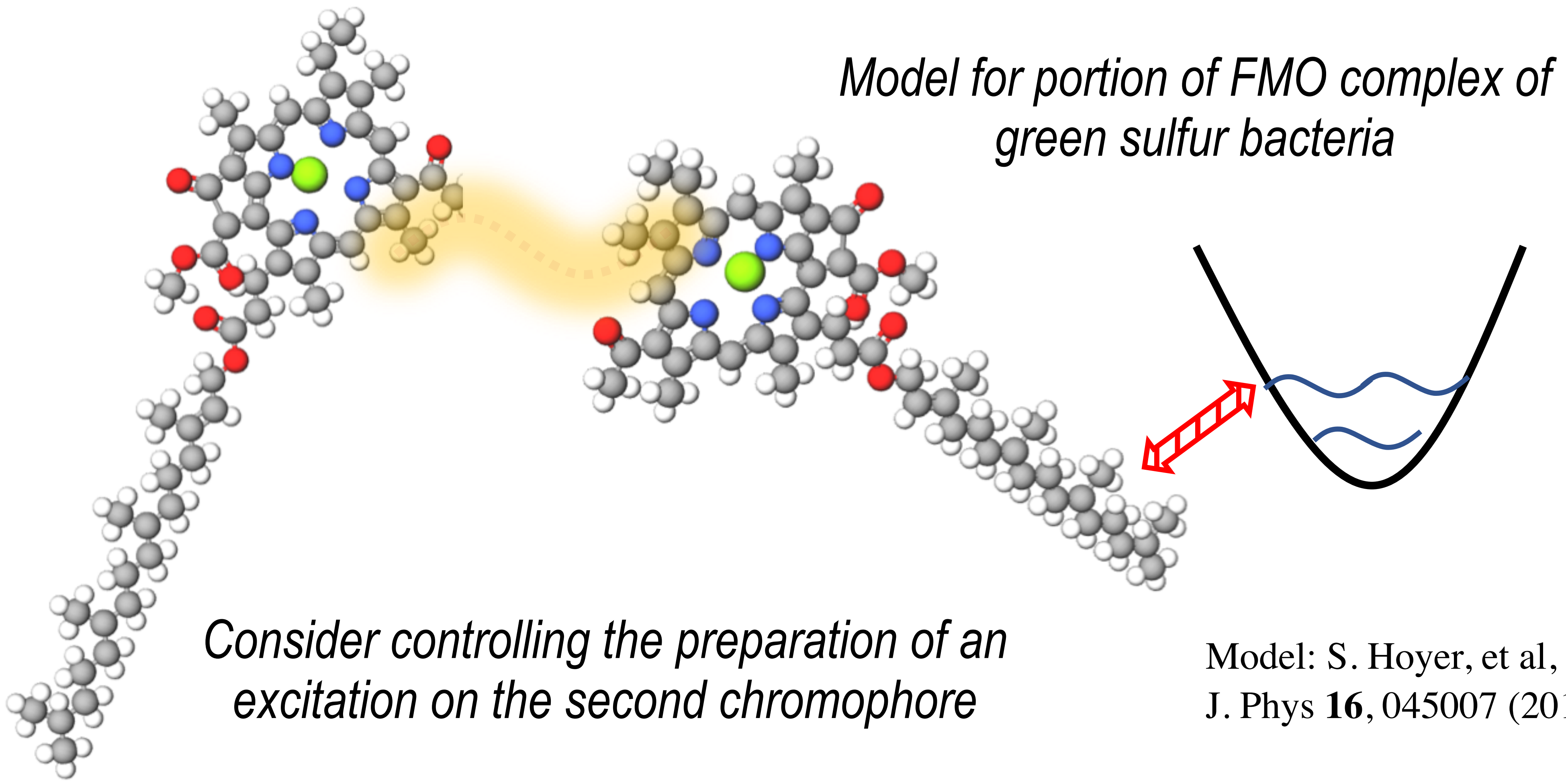
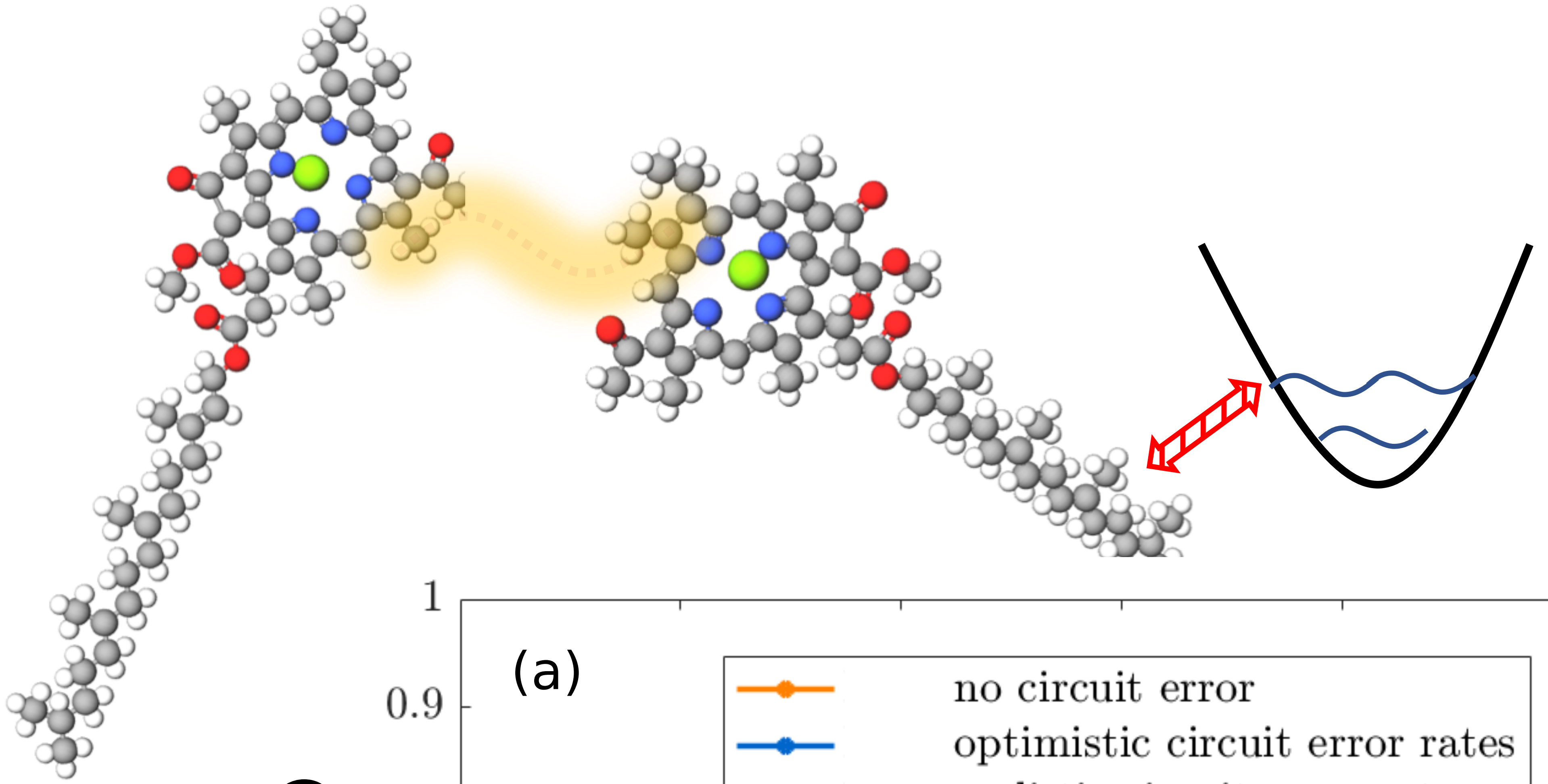
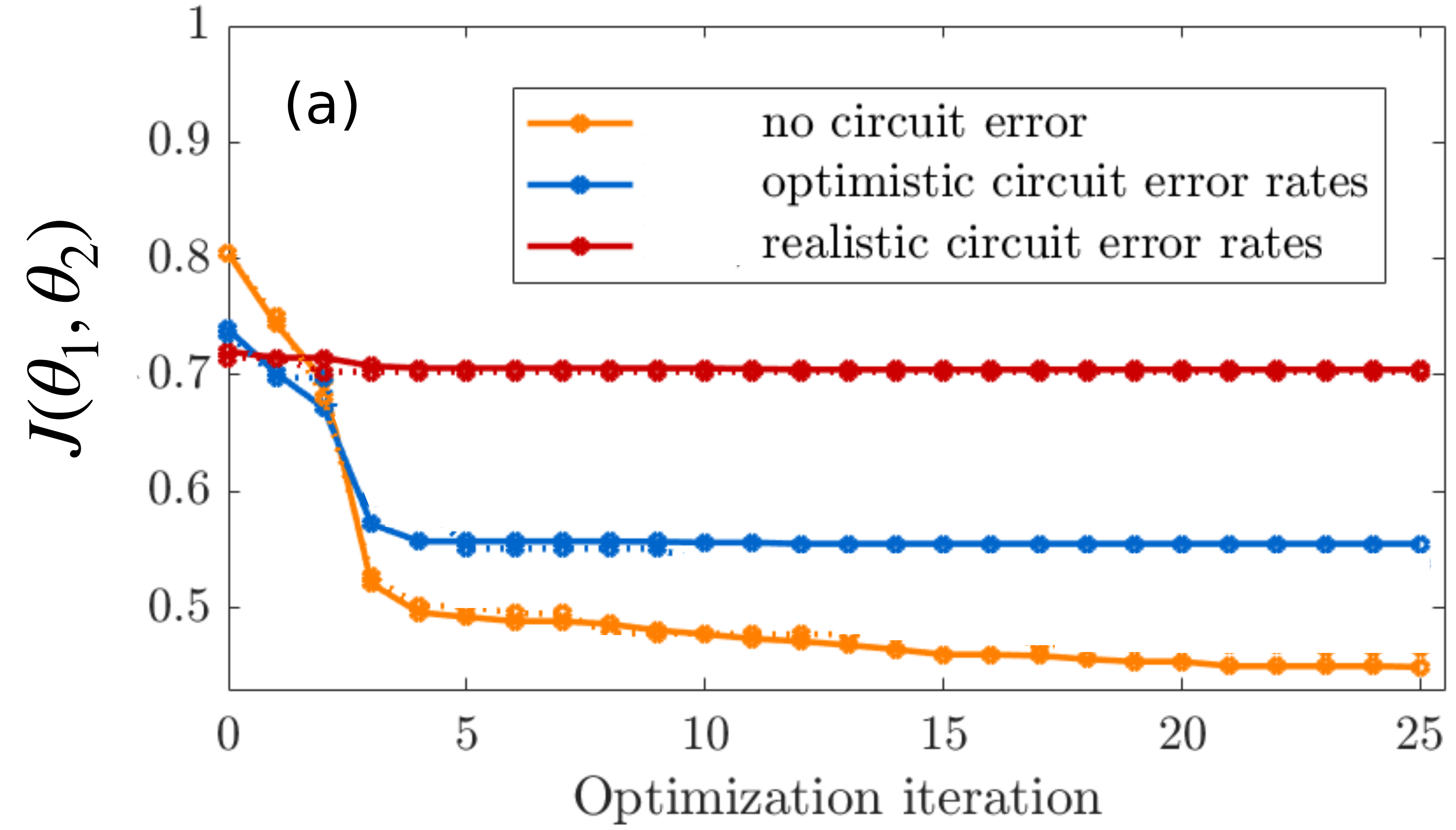
Controlled excitonic state preparation in light harvesting complex



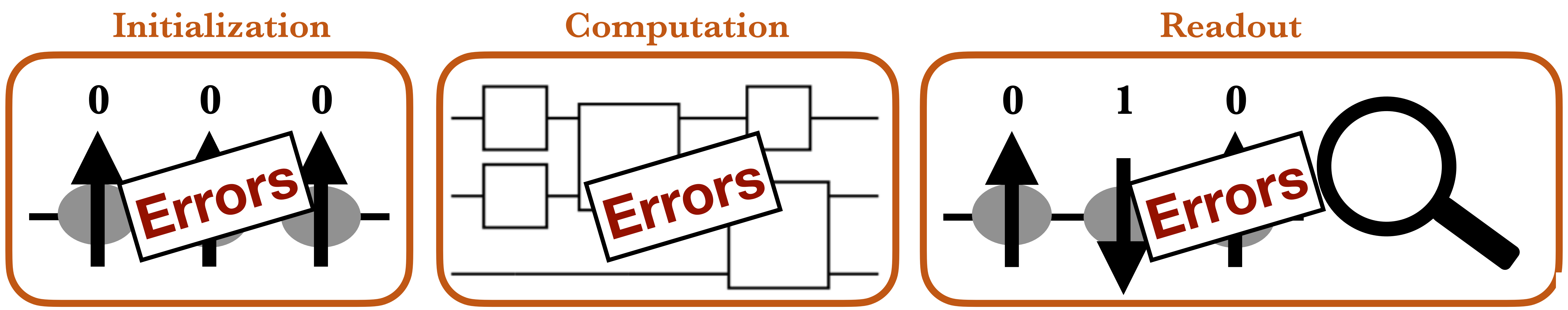
Model: S. Hoyer, et al, New J. Phys **16**, 045007 (2014).

Controlled excitonic state preparation in light harvesting complex

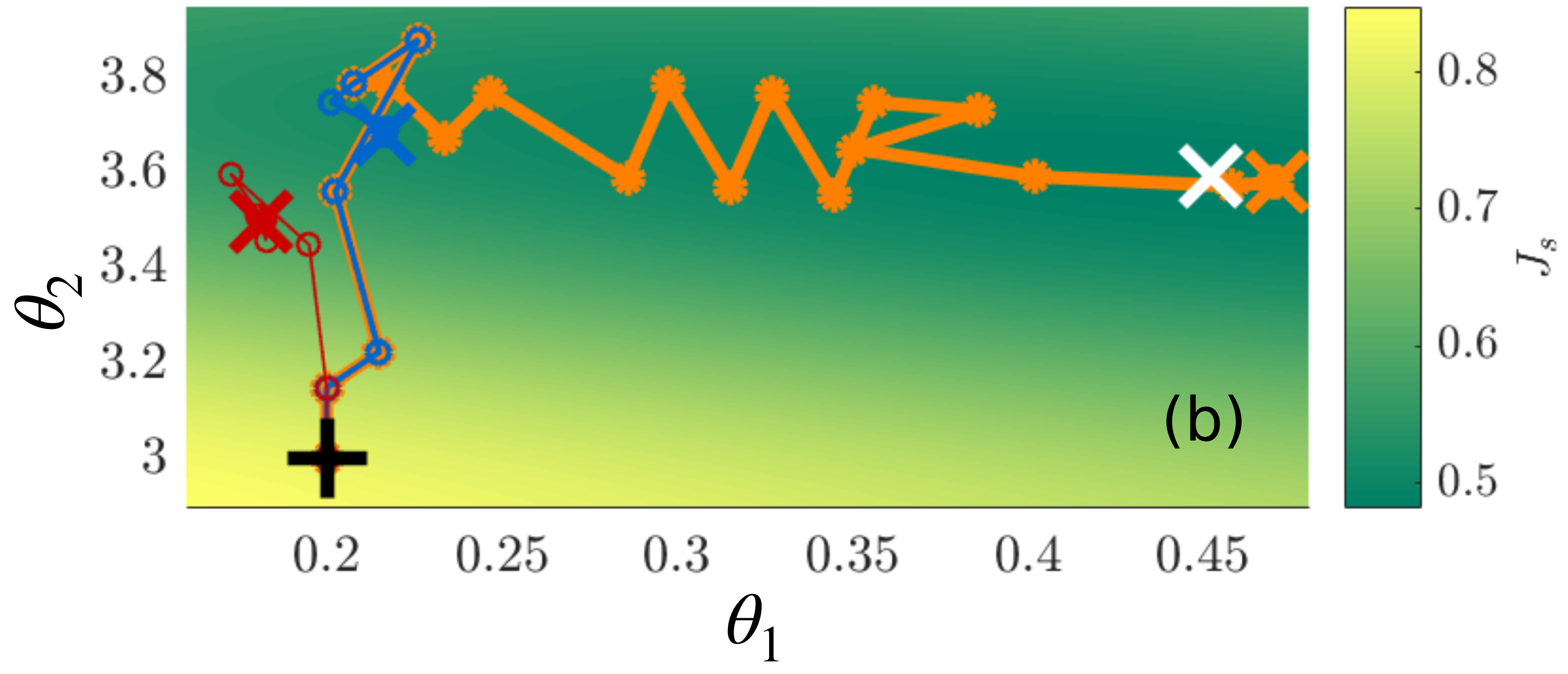




Current quantum computers are not only limited by size or speed, but also by errors

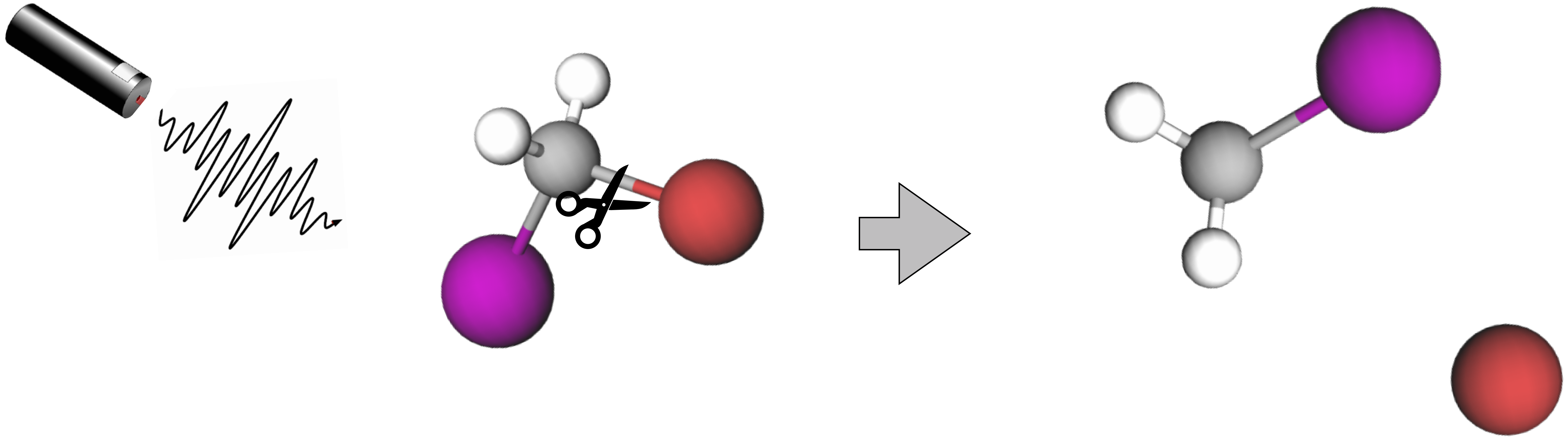


Trout, Colin J., et al. *New Journal of Physics* 20.4 (2018): 043038



We numerically explored the feasibility of meaningful implementation on error-prone trapped ion quantum hardware

Summary



- Quantum optimal control simulations involving molecular systems are notoriously challenging
    - Curse of dimensionality
- The advent of quantum computing has the potential to enable simulations of controlled molecular dynamics in polynomial time
- This talk introduced a hybrid quantum-classical algorithm for designing optimal laser fields for controlling molecular dynamics
    - Explored applications to state preparation in light harvesting complexes
    - Performed feasibility study for algorithm implementation on near-term quantum computers

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Thank you

"If you want to make a simulation of Nature, you'd better make it quantum mechanical"

Richard Feynman

DOE CSGF

Matthew Grace

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