Variational quantum algorithms: adaptive and pulse-based approaches

Sophia Economou

QTML, Melbourne, Nov 2024

Outline

- Adaptive quantum algorithms (ADAPT-VQA)
  - Background & ADAPT-VQE
  - Adaptive Gibbs state preparation

- Control-VQE: optimizing at the pulse level

Variational Quantum Eigensolver (VQE)

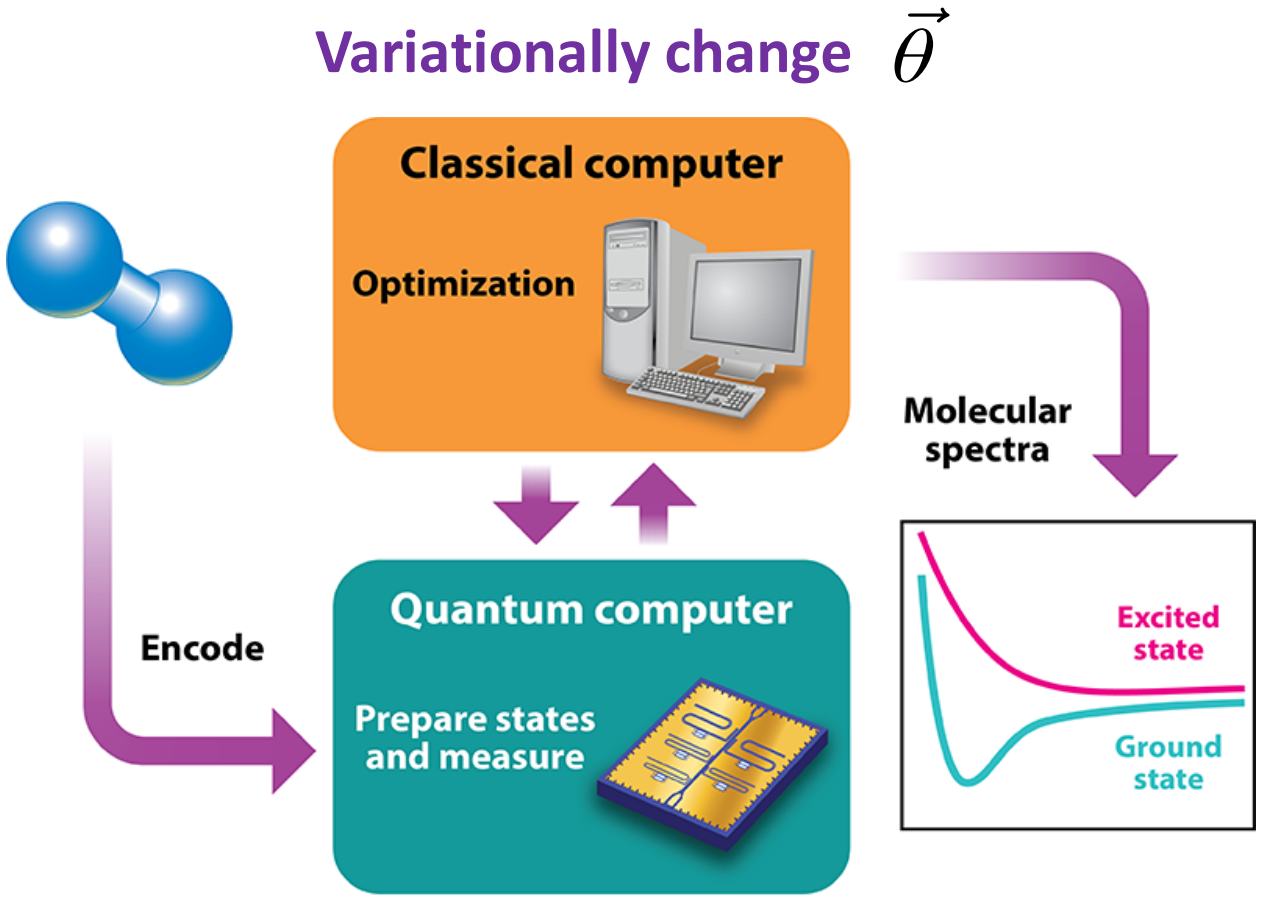
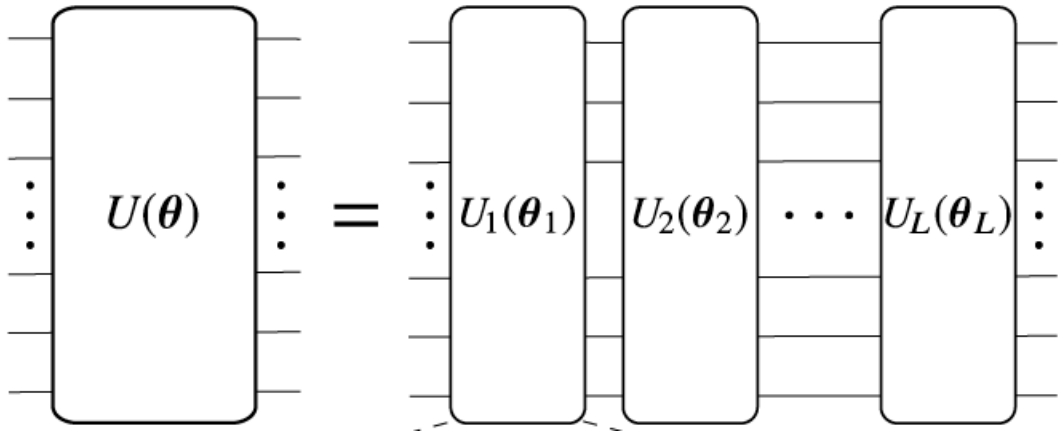


Image from Physics **11**, 14 (2018)

Ansatz $|\Psi(\vec{\theta})\rangle = U(\vec{\theta})|\Psi_{ref}\rangle$

Measured energy $E(\vec{\theta}) = \langle\Psi(\vec{\theta})|H|\Psi(\vec{\theta})\rangle$

Parametrized circuit



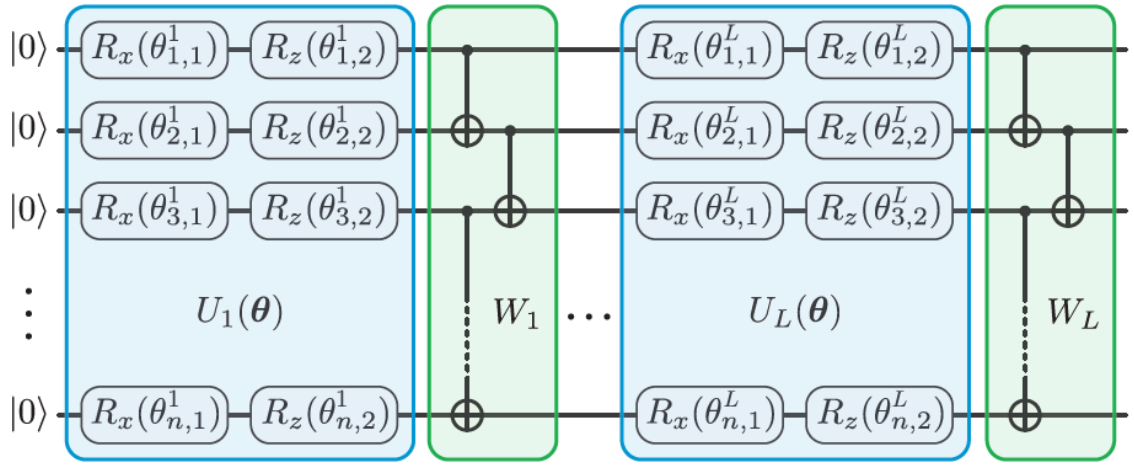
Reviews:
Cerezo et al, Nat. Rev. Phys. 3, 625 (2021)
Bharti et al, RMP 94, 015004 (2022)
Tilly et al, arXiv:2111.05176

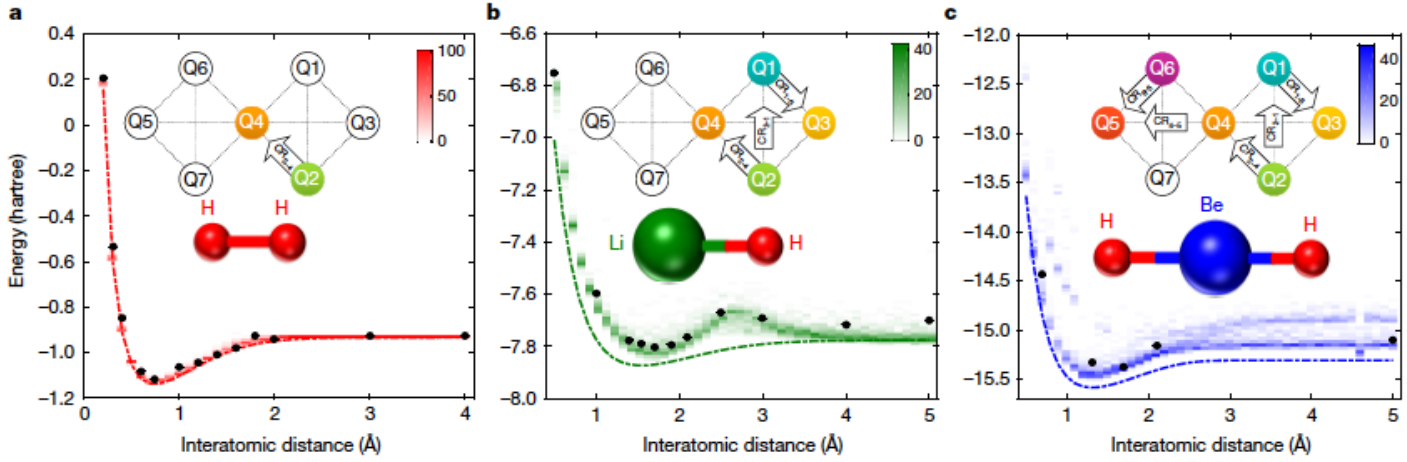
Hardware-efficient ansatz

- Tailored to chosen platform
- Inefficient—too much of the Hilbert space sampled
- *Not related to the problem* →
- Difficult to optimize (barren plateaus)

  McClean et al., Nat. Commun. 9, 4812 (2018)

  +lots of work from LANL





Kandala et al, Nature **549**, 242 (2017)

Problem-aware ansätze

- Instead of random circuits, use circuits that have knowledge of the problem
- Incorporate: symmetries (particle number, spin, spatial symmetry, etc), locality
- This can avoid issues with optimization, can lead to shorter circuits

Fermionic Hamiltonian and mapping

$$H = \sum_{p,q=1}^{N} h_{pq} a_p^\dagger a_q + \sum_{p,q,r,s=1}^{N} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

Map (spin) orbitals to qubits: Jordan-Wigner mapping

$$a_i^\dagger \mapsto \frac{1}{2}(X_i - \mathrm{i}Y_i) \prod_{r=0}^{i-1} Z_r \qquad a_i \mapsto \frac{1}{2}(X_i + \mathrm{i}Y_i) \prod_{r=0}^{i-1} Z_r$$

Z strings O(*N*)

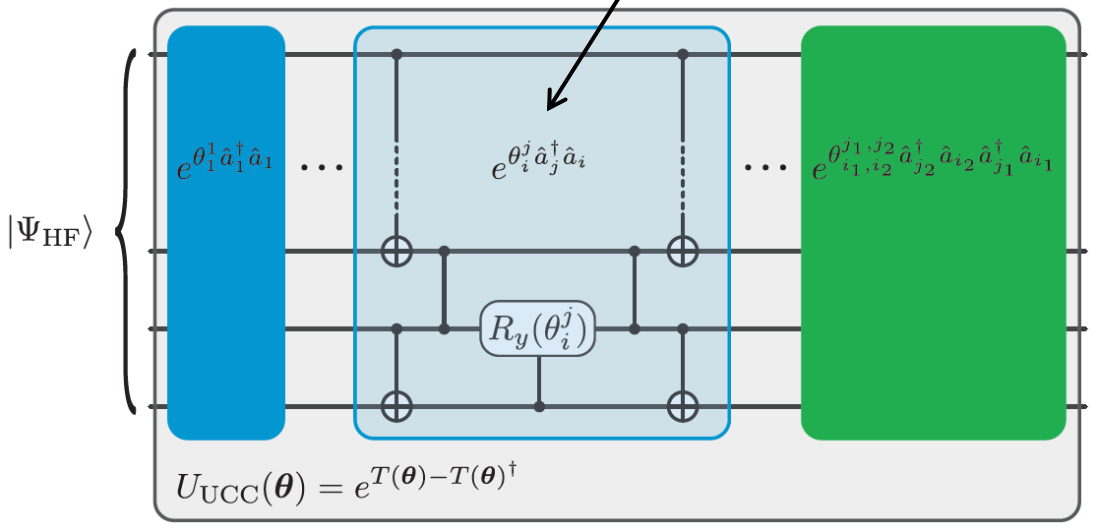
One of the first problem-aware ansätze: UCCSD

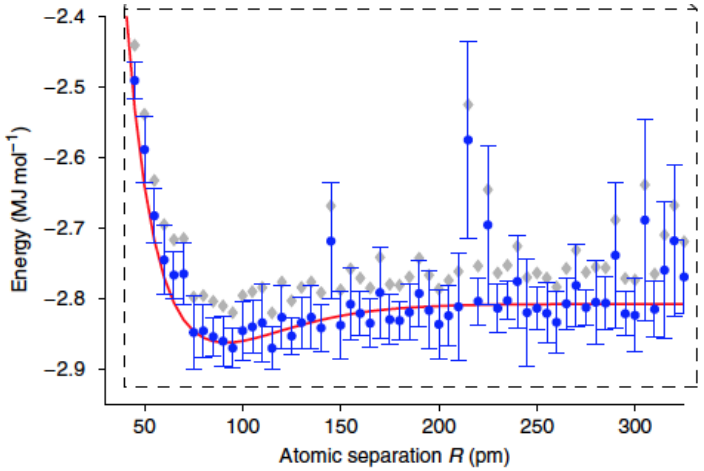
gates built from symmetry-adapted fermionic operators

Chemistry-inspired (UCCSD) ansatz

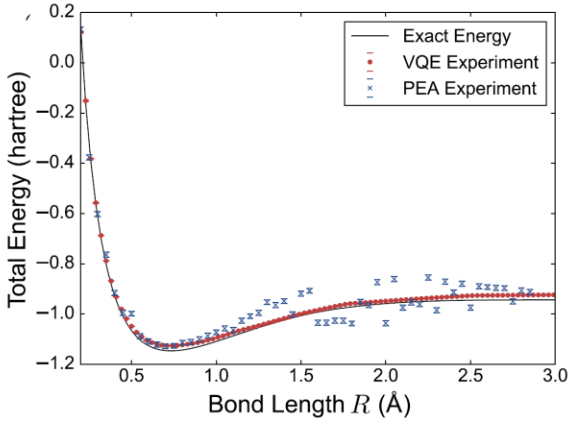
- Incorporates symmetries
- Generalizes classical simulations
- Impractically long circuits, many CNOTs
- Inconsistent under low-order Trotterization

Grimsley et al., JCTC 2020, 16, 1, 1-6

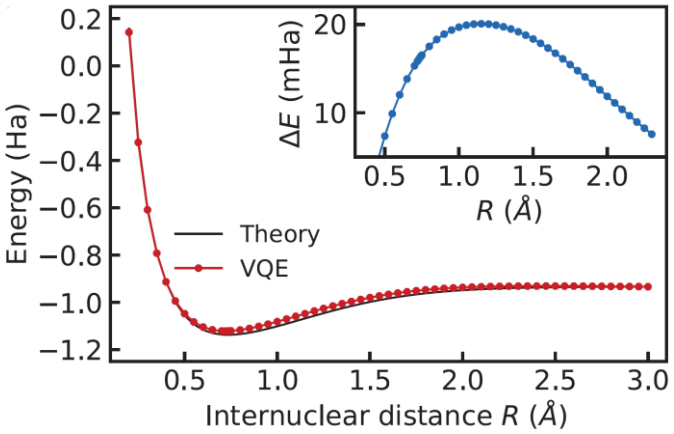




*Peruzzo et al, Nature Comm. **5**, 1 (2014)*



*O'Malley et al, PRX **6**, 031007 (2016)*



Xue et al, Nature 601, 343 (2022)

Constructing ansatz: desiderata

Quantum circuit that is:

- Short
- Expressive
- Trainable

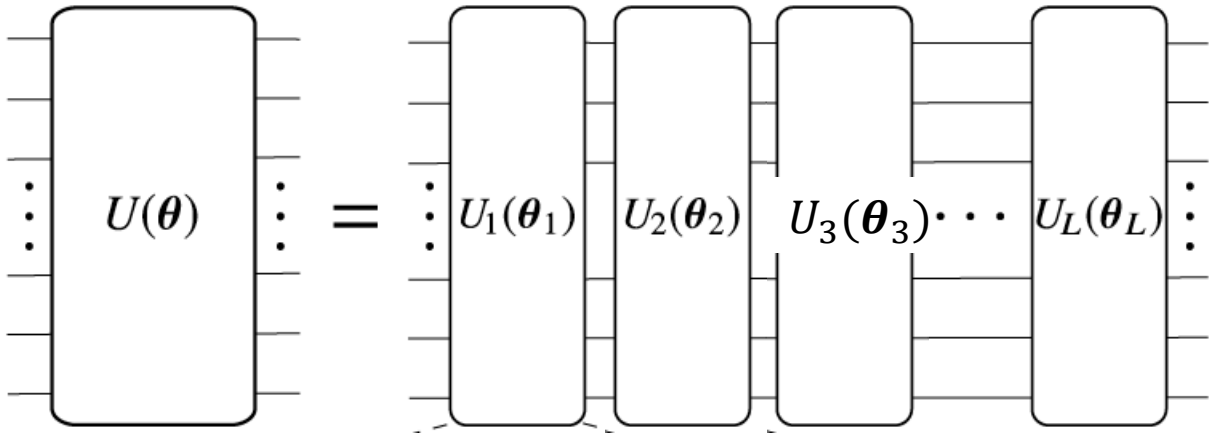
Outline

- Adaptive quantum simulation (ADAPT-VQE)
  - Molecules
  - Periodic systems

- Control-VQE: optimizing at the pulse level

Adaptive, problem-tailored VQE (ADAPT-VQE)

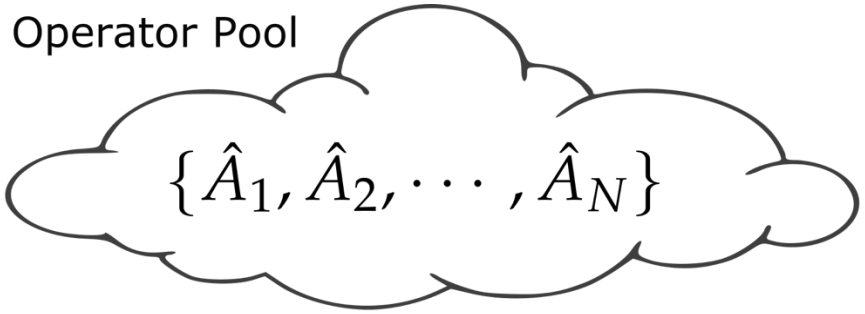
- Start from a simple reference state
- Quantum resources are precious: Only add as many operators as needed
- Problem-tailor the ansatz: Use the QC to determine how to grow the ansatz further



Grimsley, Economou, Barnes, Mayhall, Nature Communications **10**, 3007 (2019)

ADAPT-VQE ingredients: (i) operator pool

- ADAPT-VQE uses a pool of operators, A_m
- Applies unitaries one by one : $U_m = \exp(\theta_m A_m)$ to a reference state



Grimsley, Economou, Barnes, Mayhall, Nature Communications **10**, 3007 (2019)

ADAPT-VQE ingredients: (ii) update criterion

- Identify which $e^{\theta_j A_j}$ to apply to reference state $|\Psi_0\rangle$
- Take gradient of mean energy wrt θ_j

$$\frac{\partial}{\partial \theta_j} \langle \Psi_k | e^{-\theta_j A_j} H e^{\theta_j A_j} | \Psi_k \rangle |_{\theta_j = 0} = \langle \Psi_k | \underbrace{[H, A_j]} | \Psi_k \rangle$$

New operator → measure on hardware

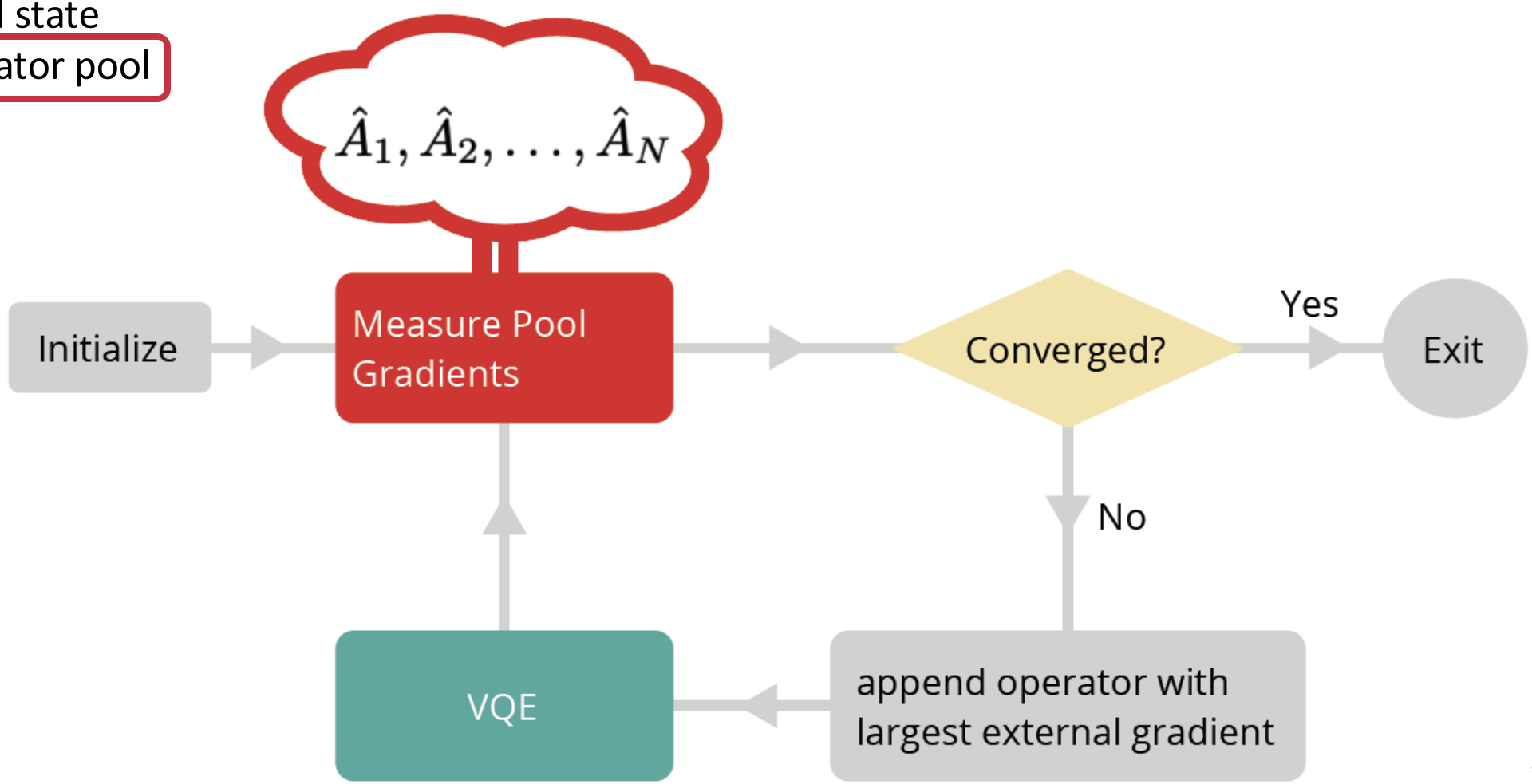
k: ADAPT iteration step

Grimsley, Economou, Barnes, Mayhall, Nature Communications **10**, 3007 (2019)

ADAPT-VQE overview

Inputs:

- Hamiltonian
- Initial state
- Operator pool



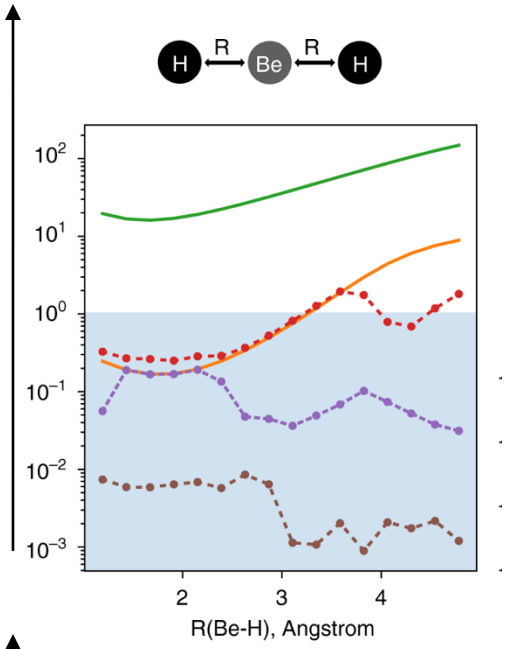
Grimsley, Economou, Barnes, Mayhall, Nature Communications **10**, 3007 (2019)

ADAPT-VQE with fermionic pool

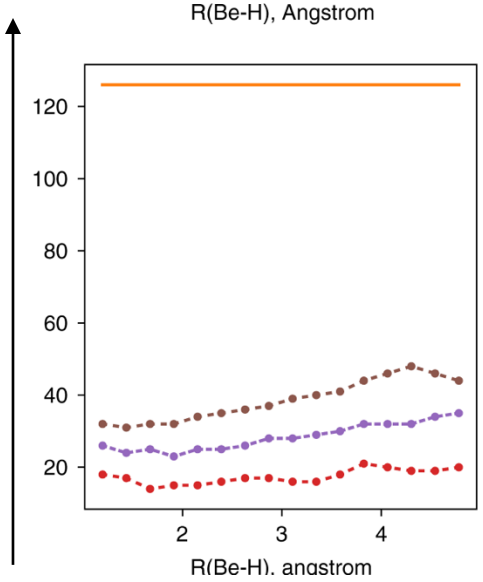
UCCSD
HF
ADAPT(ϵ_1)
ADAPT(ϵ_2)
ADAPT(ϵ_3)
Chemical Accuracy

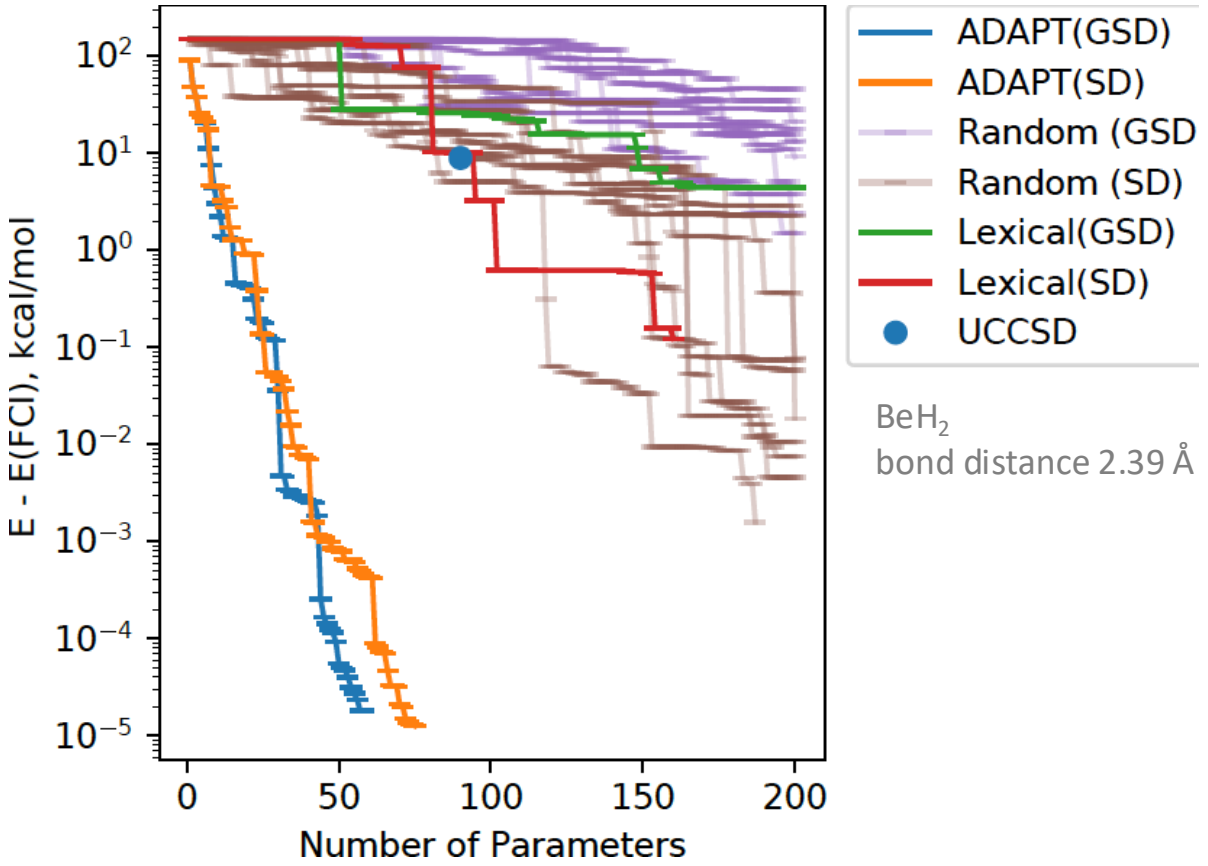
$\epsilon_1 = 0.1$
$\epsilon_2 = 0.01$
$\epsilon_3 = 0.001$

energy error



nr of variational parameters





BeH_2
bond distance 2.39 Å

Grimsley, Economou, Barnes, Mayhall,
Nature Communications **10**, 3007 (2019)

ADAPT-VQE vs other ansätze

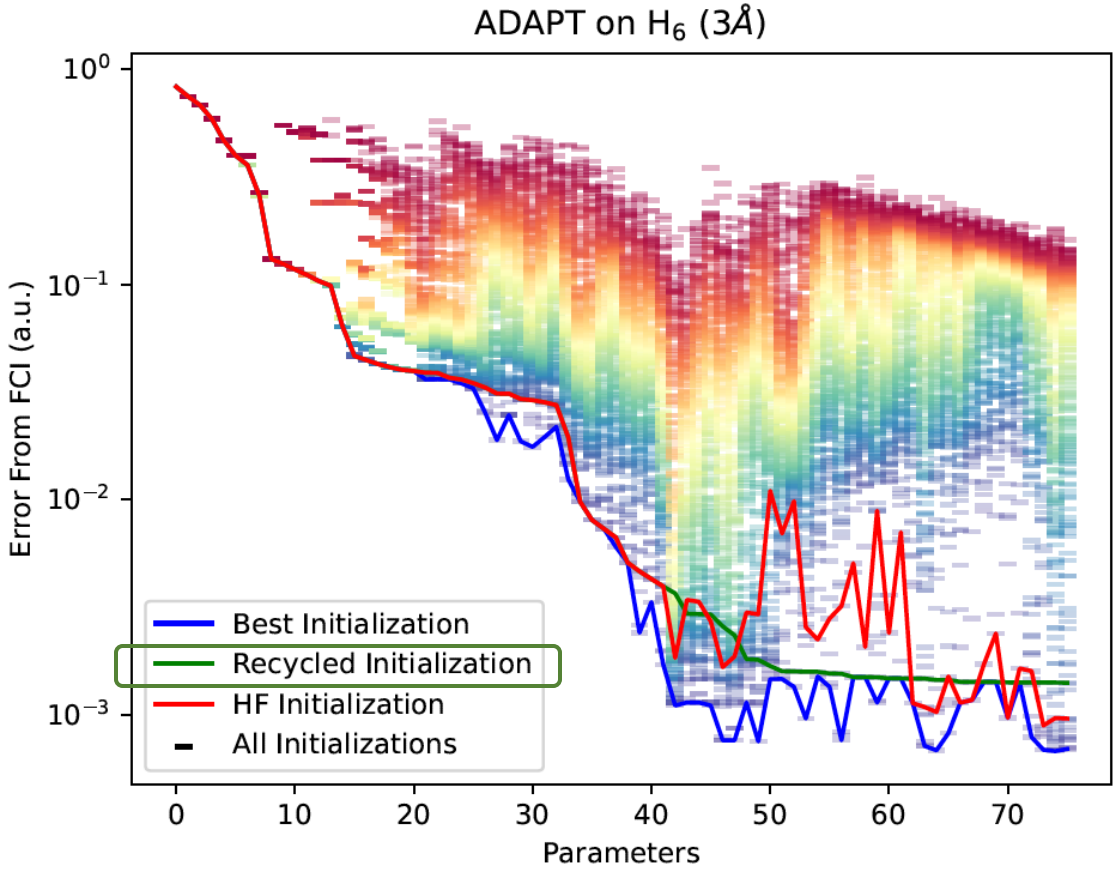
***Problem-tailored* vs problem-aware**

Example: ansatz at different points on dissociation curve of a given molecule

- UCCSD: exact same across curve
- ADAPT-VQE: changes across the curve, picks up operators as needed for strongly correlated regions

Trainability of ADAPT-VQE

- ADAPT produces compact tailored ansätze
- Shallow circuit → the landscape is generally too rugged
- ADAPT avoids the issues associated with trainability
- By construction resistant to barren plateaus



Grimsley et al, npj Quantum Information **9**, 19 (2023)

ADAPT-VQE vs other ansätze

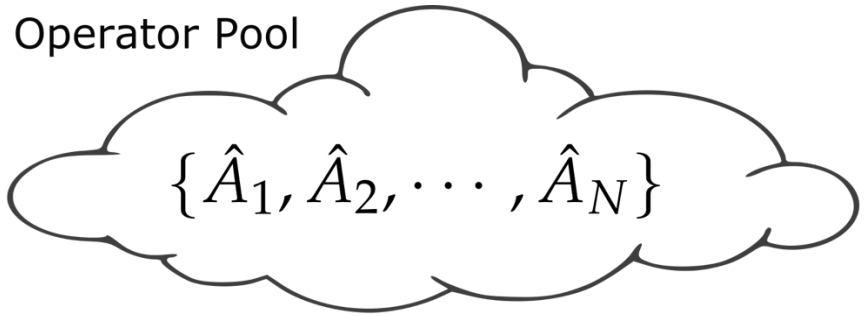
- ***Problem-tailored* vs problem-aware**

  Example: ansatz at different points on dissociation curve of a given molecule

  - UCCSD: exact same across curve
  - ADAPT-VQE: changes across the curve, picks up operators as needed for strongly correlated regions

- ***Expressivity potential* vs expressive circuits**
  - Random circuits: very expressive, hard to optimize
  - ADAPT-generated ansatz:
    - bespoke to problem, each instance not random
    - parameters warm-started

How should the operator pool be chosen?



Criteria & desiderata

- Problem constraints: **symmetries**, etc
- Hardware constraints: **connectivity, locality**, etc
- Small pool size
- …

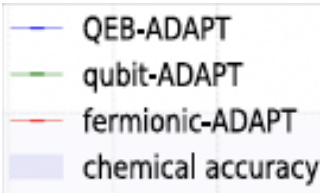
An obvious choice is the ***fermionic pool***

- Preserves particle number
- Can be spin-adapted (preserves Sz)

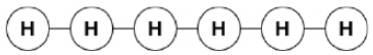
But:

- Hardware inefficient
- Grows with system size

ADAPT-VQE: Pool Choices

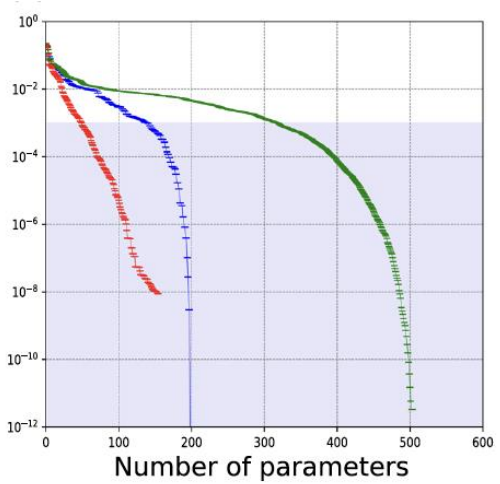


The choice of operator pool impacts the circuit- and parameter-efficiency of the final ansatz. Popular pool types include:



- Fermionic Pools: Operators directly correspond to fermionic excitations

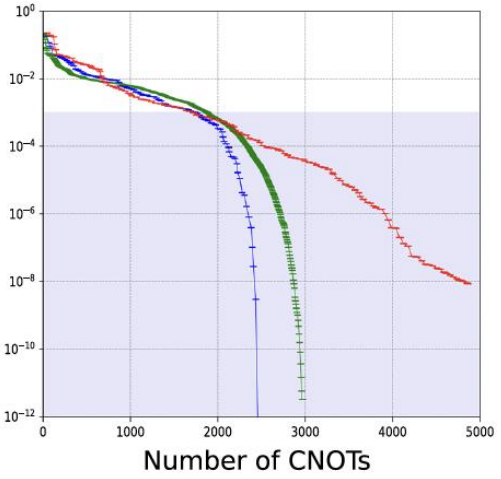
$$T_{ijkl} \equiv a_i^\dagger a_j^\dagger a_k a_l - a_k^\dagger a_l^\dagger a_i a_j$$



- Qubit Excitation (QE) Pools: Operators correspond to fermionic excitations up to anticommutation effects

$$\tilde{T}_{ijkl} \equiv Q_i^\dagger Q_j^\dagger Q_k Q_l - Q_k^\dagger Q_l^\dagger Q_i Q_j$$

(h)



- Qubit Pools: Operators are individual Pauli strings

$$i \cdot Y_q X_p X_s X_r, \quad i \cdot X_q Y_p X_s X_r, \quad i \cdot X_q X_p Y_s X_r, \quad i \cdot X_q X_p X_s Y_r,$$
$$i \cdot X_q Y_p Y_s Y_r, \quad i \cdot Y_q X_p Y_s Y_r, \quad i \cdot Y_q Y_p X_s Y_r, \quad i \cdot Y_q Y_p Y_s X_r.$$

Yordanov et al, *Commun Phys* **4**, 228 (2021)
Tang et al, *PRX Quantum* **2**, 020310 (2021)

We can do even better by further incorporating symmetries: Coupled-excitation operator pool

Couple certain excitations based on symmetry considerations

E.g., QE pool does not take $\alpha_1, \beta_1 \rightarrow \alpha_2, \beta_2$ on the same footing as $\alpha_1, \beta_2 \rightarrow \alpha_2, \beta_1$ (α: spin up; β: spin down)

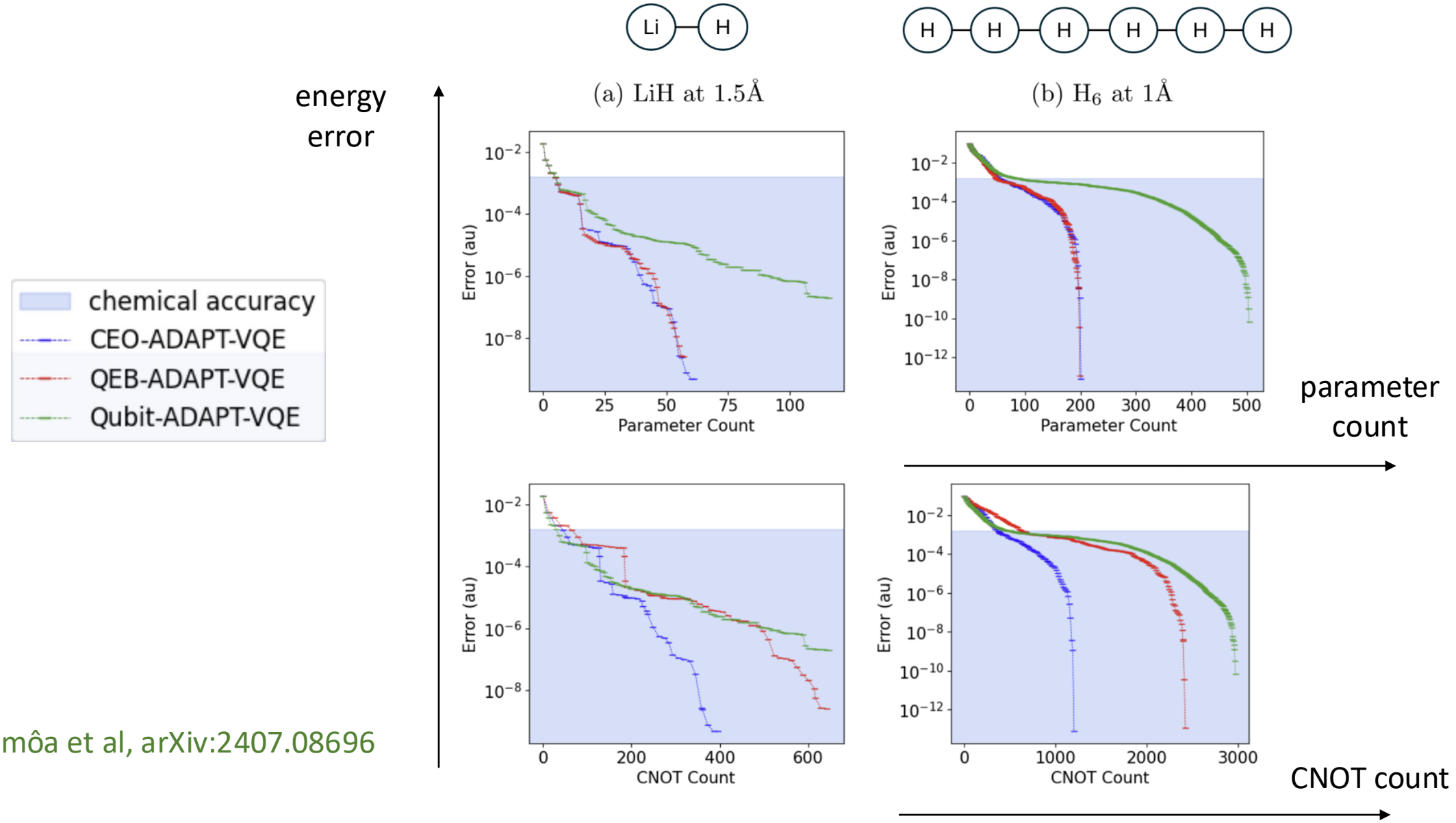
If we couple such operators, we obtain a pool with operators of the form:

$$T^{(MVP-CEO)}_{\alpha_1\beta_1\alpha_2\beta_2}(\theta_1,\theta_2) =$$
$$\frac{i}{8}[+(\theta_1+\theta_2)XXXY-(\theta_1+\theta_2)XXYX$$
$$+(\theta_1-\theta_2)XYXX+(\theta_1-\theta_2)XYYY$$
$$-(\theta_1-\theta_2)YXXX-(\theta_1-\theta_2)YXYY$$
$$+(\theta_1+\theta_2)YYXY-(\theta_1+\theta_2)YYYX].$$

Ramôa et al, arXiv:2407.08696

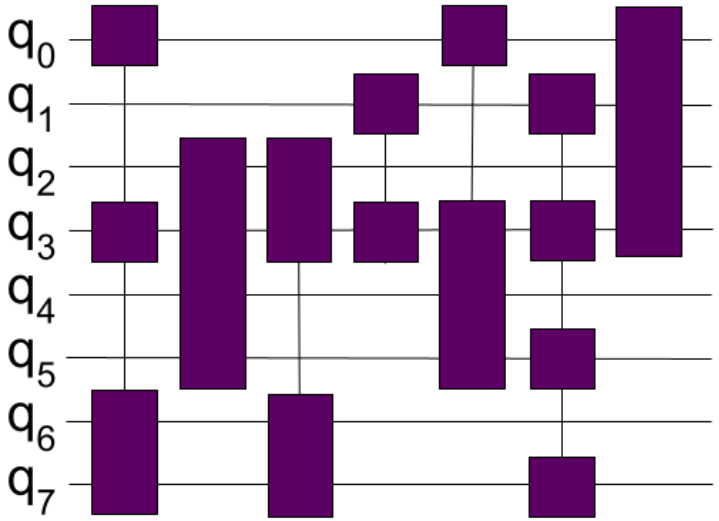
See Mafalda's talk at 4.15 pm

CEO pool, results & comparison to qubit and QE pools



Ramôa et al, arXiv:2407.08696

- Is ADAPT-VQE the most efficient way to construct circuits?
- Can we optimize further for circuit depth?

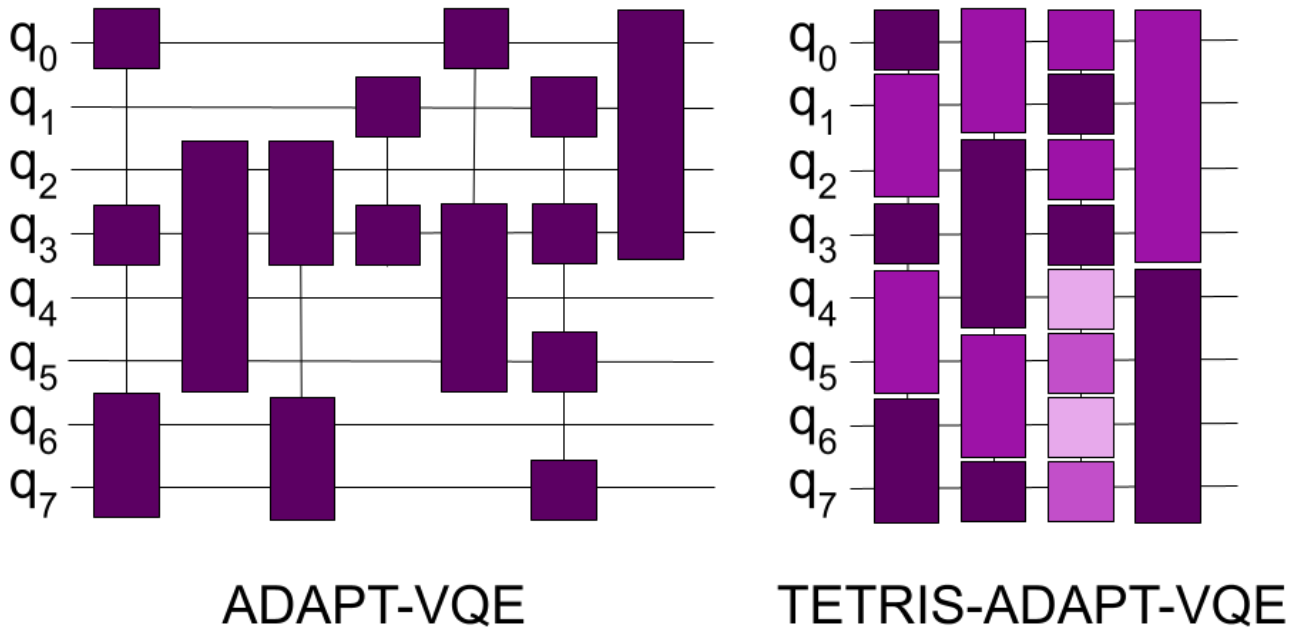


ADAPT-VQE

TETRIS-ADAPT-VQE: concept

Tiling Efficient Trial circuits with Rotations Implemented Simultaneously

Instead of one-at-a-time, add multiple operators at each step



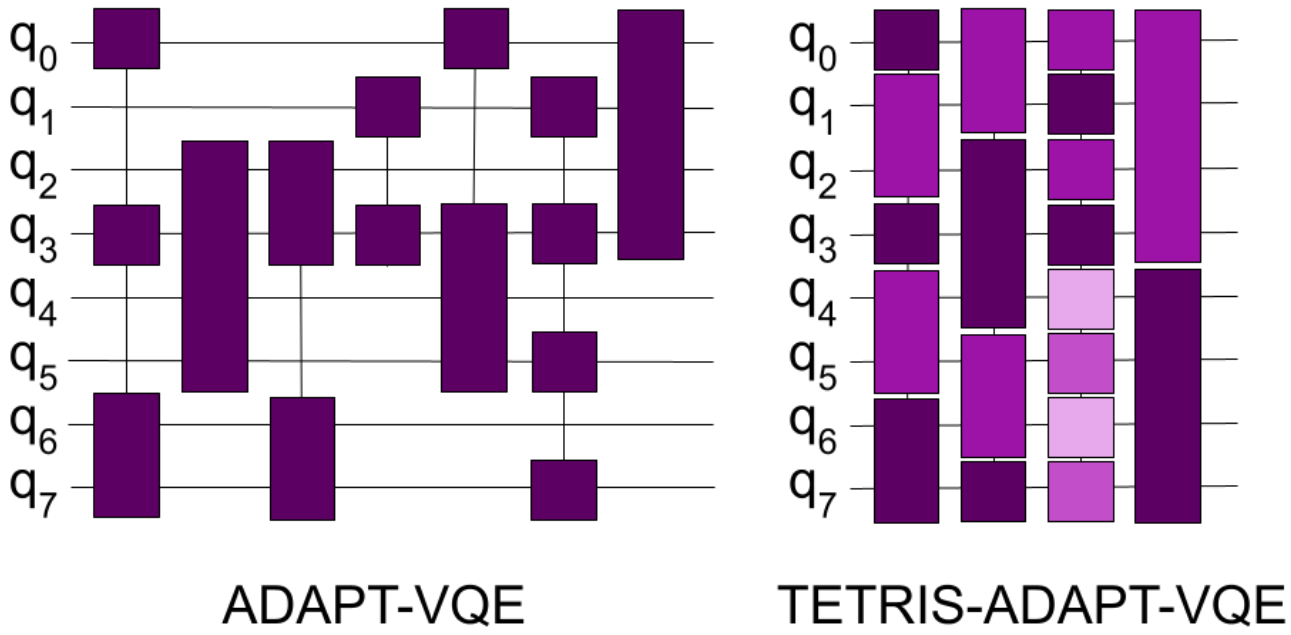
Anastasiou, et al Phys. Rev. Research 6, 013254 (2024)

TETRIS-ADAPT-VQE: concept

Tiling Efficient Trial circuits with Rotations Implemented Simultaneously

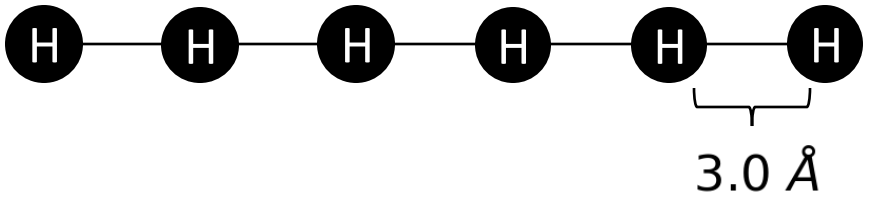
Instead of one-at-a-time, add multiple operators at each step according to:

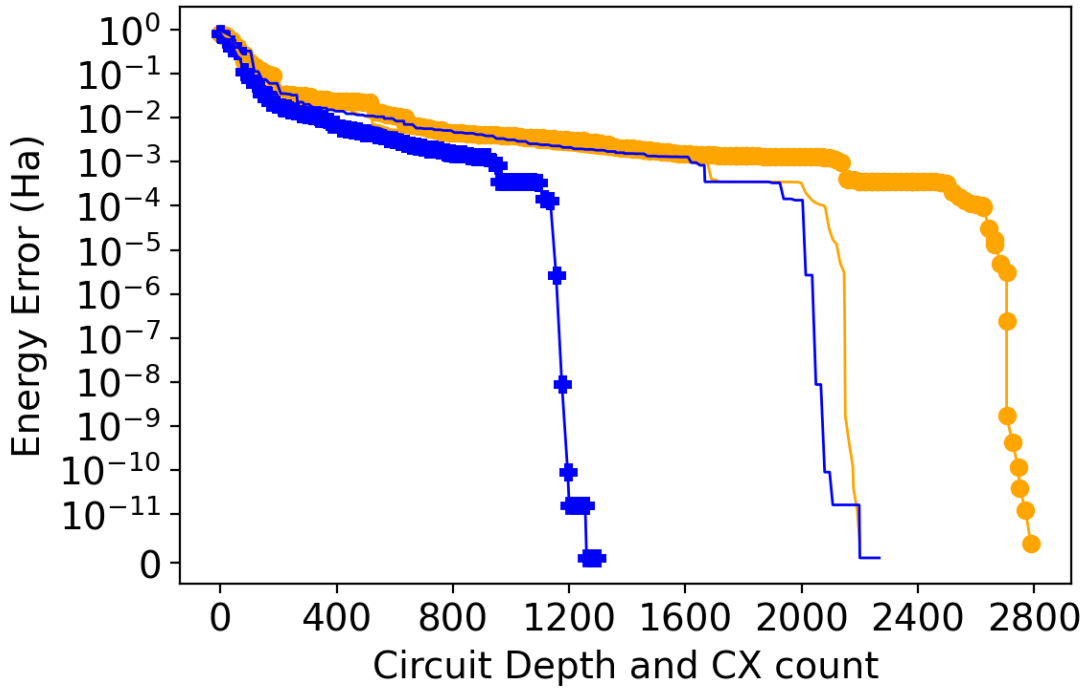
- Gradient magnitude
- $\mathcal{N}$th operator acting on different set of qubits from $(\mathcal{N}-j)$th



Anastasiou, et al Phys. Rev. Research 6, 013254 (2024)

TETRIS-ADAPT-VQE: results



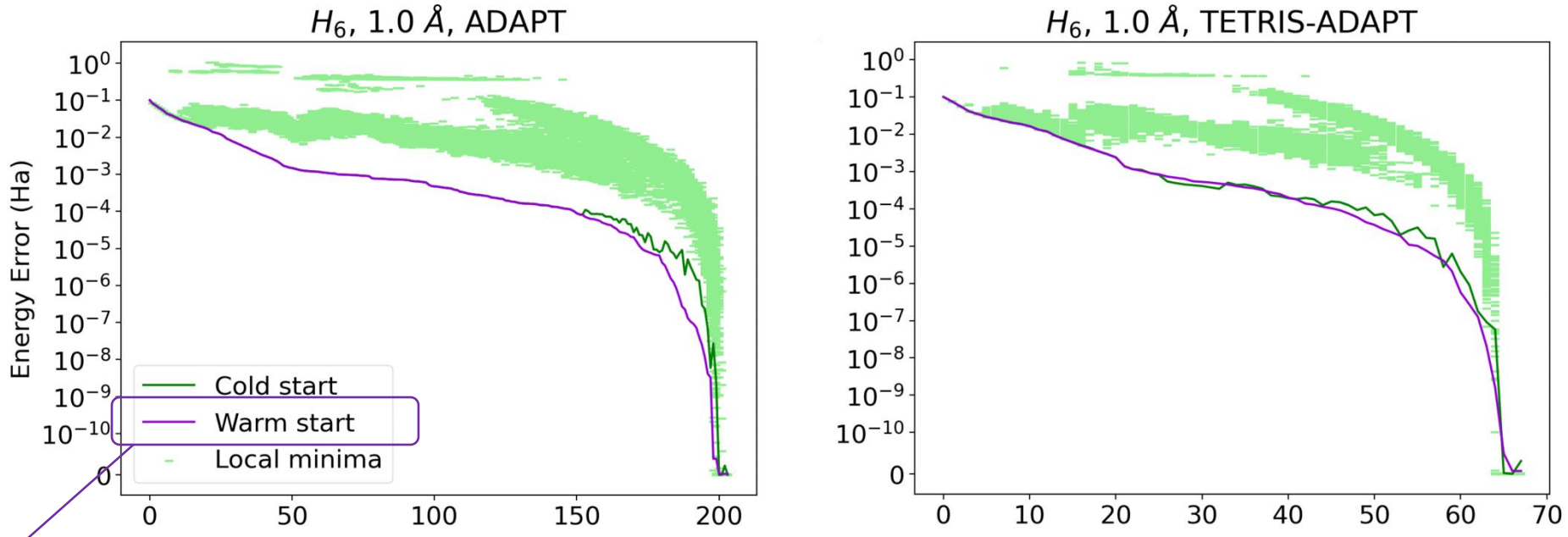


Blue: TETRIS-ADAPT

Orange: standard ADAPT

Anastasiou, et al Phys. Rev. Research 6, 013254 (2024)

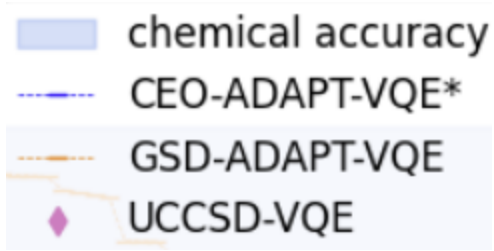
Trainability of TETRIS-ADAPT-VQE



ADAPT strategy

Anastasiou, et al Phys. Rev. Research 6, 013254 (2024)

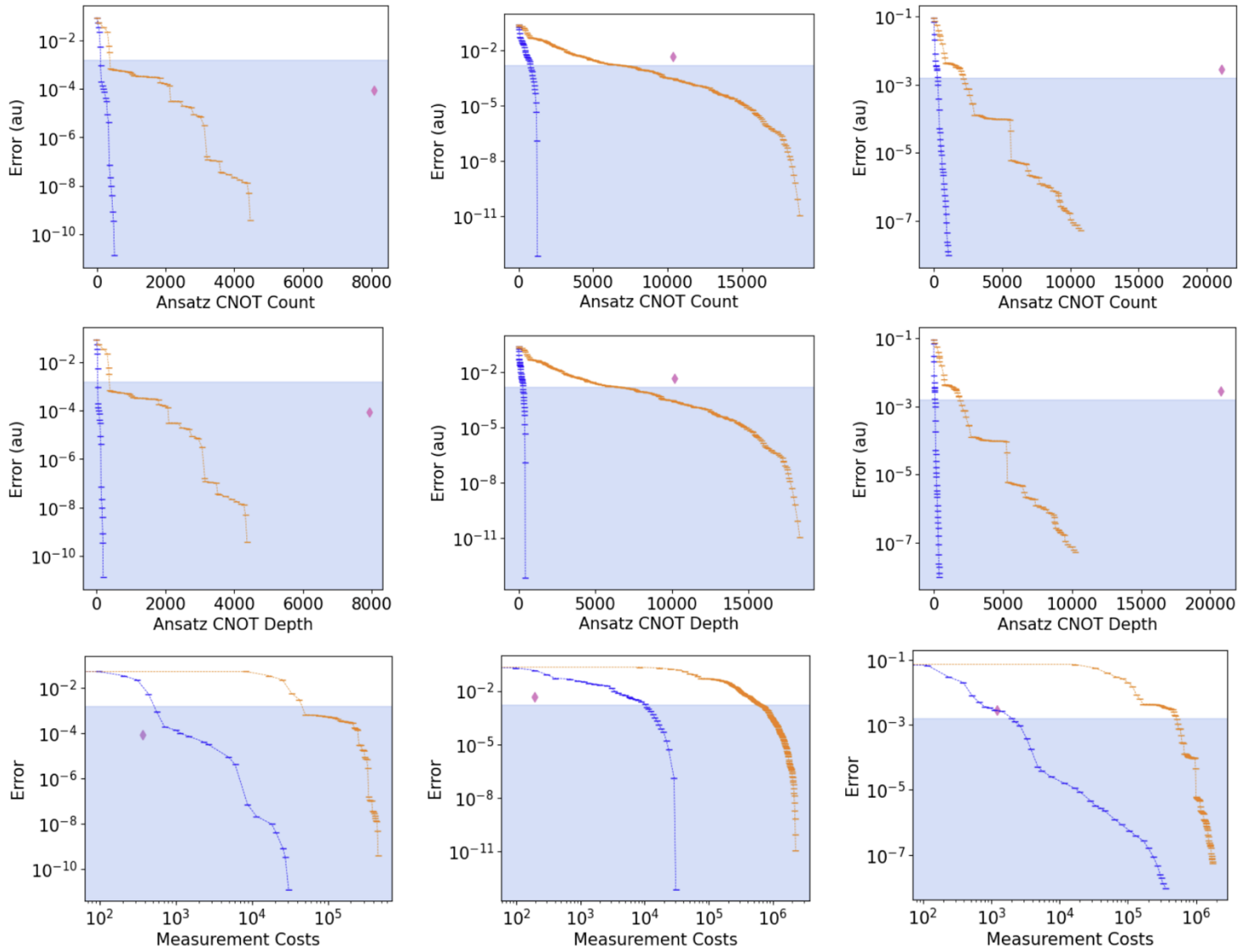
Putting it all together: CEO-ADAPT-VQE*
2019 vs 2024 ADAPT-VQE



- New (CEO) pool
- TETRIS strategy
- Recycling Hessian
- Grouping commuting operators

Compared to UCCSD:

- Order(s) of magnitude improvement in CNOT count/depth
- Comparable nr of measurements



(a) LiH at 3Å (b) H_6 at 1.5Å (c) BeH_2 at 2Å

Outline

- Adaptive quantum algorithms (ADAPT-VQA)
  - Background & ADAPT-VQE
  - Adaptive Gibbs state preparation
- Control-VQE: optimizing at the pulse level

Gibbs state preparation

- Given Hamiltonian H acting on data system D with N_D qubits, we wish to prepare mixed thermal states at arbitrary temperature T

$$\rho_G(T) = \frac{e^{-H/T}}{\mathrm{Tr}(e^{-H/T})}$$

- This has useful applications in quantum simulation, quantum machine learning, quantum optimization, etc., but is a hard problem in general

- Standard approach: prepare state that minimizes $F\left(\rho(\vec{\theta})\right) = \mathrm{Tr}\left(\rho(\vec{\theta})H + T\rho(\vec{\theta})\ln\rho(\vec{\theta})\right)$

- Challenges:
  - It's hard to know *a priori* what will make an efficient, effective ansatz
  - Measuring the entropy (and gradients) is difficult on hardware

Wu and Hsieh. PRL **123**, 220502 (2019)
Chowdhury, Low, and Wiebe. arXiv:2002:00055 (2020)
Wang, Li, and Wang. PRA **16**, 054035 (2021)

Gibbs-ADAPT-VQE

- Our approach:
  - ✓New objective function that is easier to measure:

$$C\left(\rho\left(\vec{\theta}\right)\right) = -\operatorname{Tr}\left(\rho_G(T)\rho\left(\vec{\theta}\right)\right) + \frac{1}{2}\operatorname{Tr}\left(\rho\left(\vec{\theta}\right)^2\right)$$

  - ✓ADAPT-VQE approach to grow the ansatz

Warren et al, arXiv: 2203.12757

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  - ✓ADAPT-VQE approach to grow the ansatz

- Ancilla system can be any size, allowing resource savings (though $N_A = N_D$ needed at larger T)

- Operator pool: all 1- and 2-qubit Pauli's on combined data/ancilla system
- Pool requires initial state be only **partially entangled** (use non-optimized random y-rotations and CNOTs)

Warren et al, arXiv: 2203.12757

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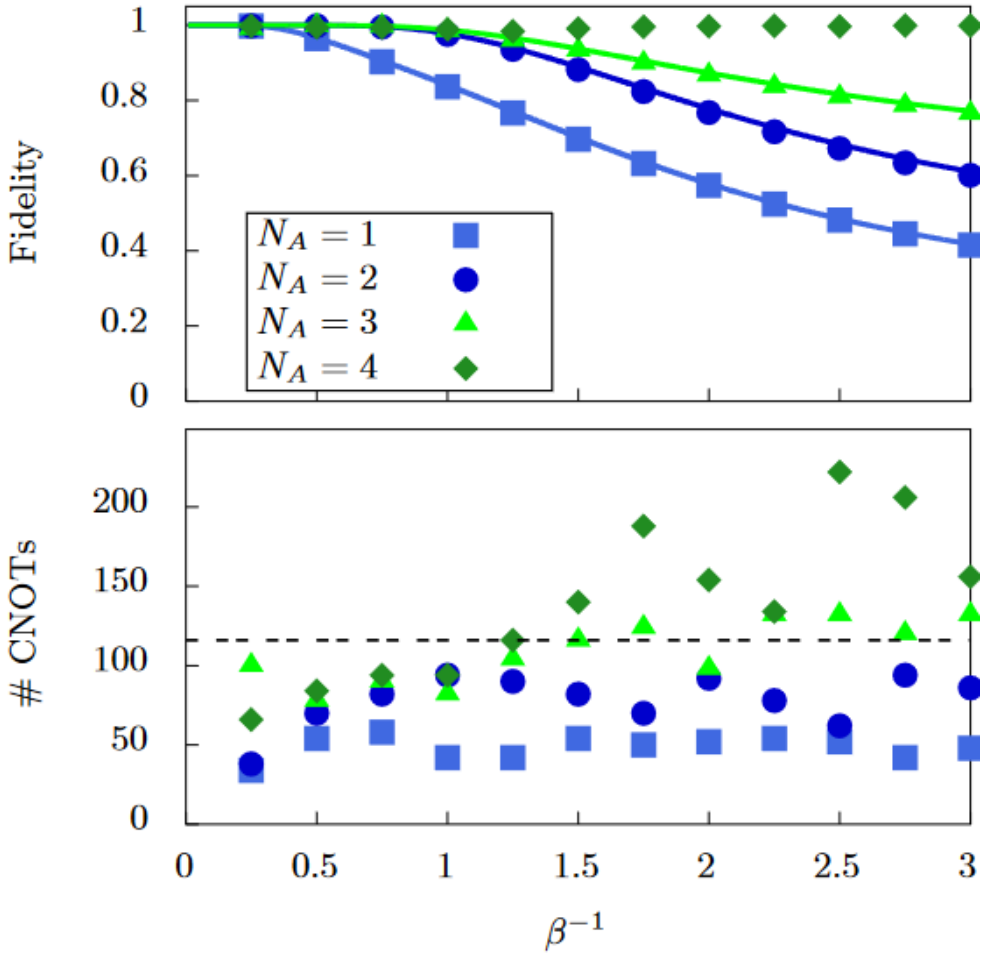
Periodic XY Hamiltonian

$$H = -\sum_{i=1}^{N_D} X_i X_{i+1} + Y_i Y_{i+1} \qquad N_D = 4$$

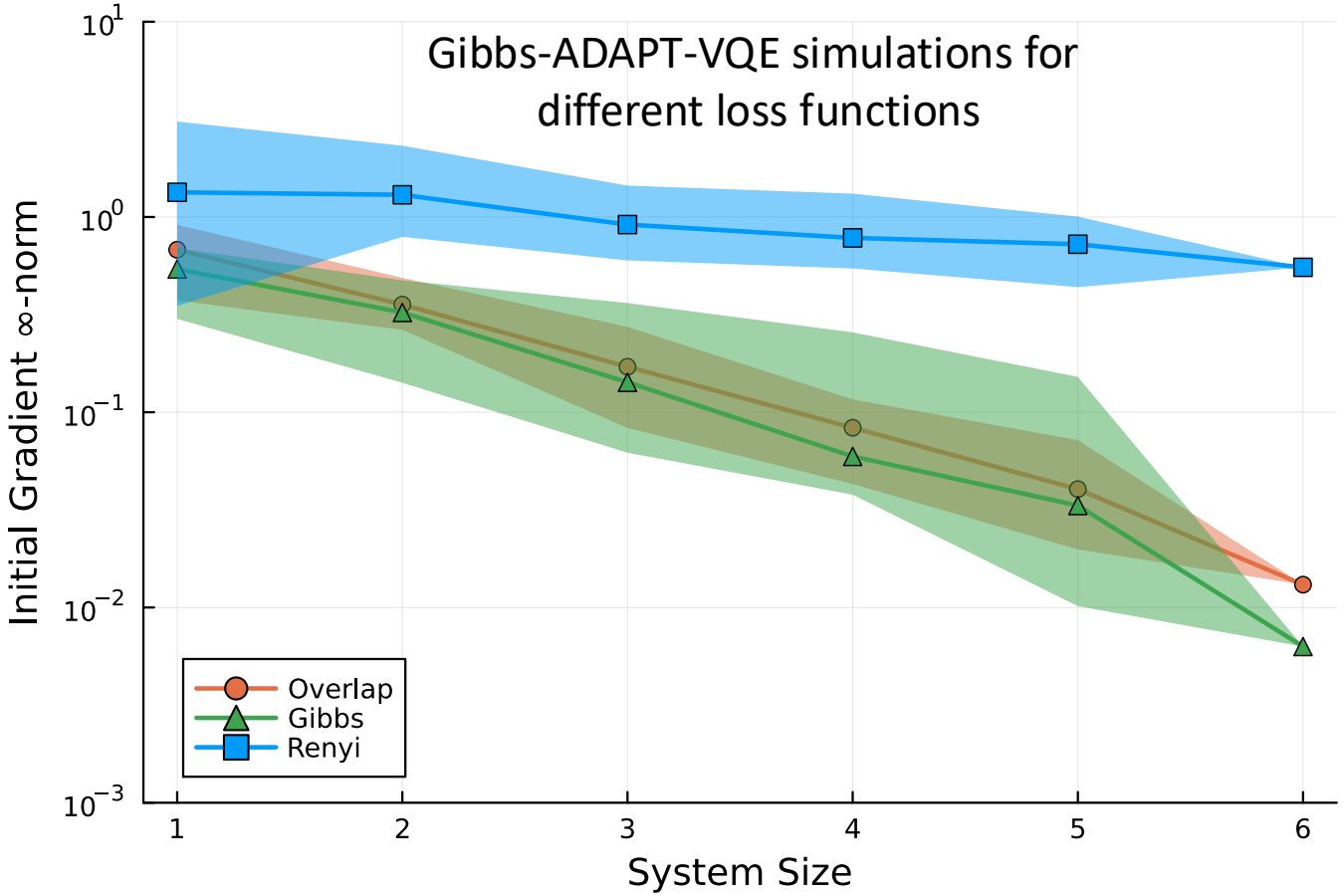


Warren et al, arXiv: 2203.12757

Avoiding barren plateaus in Gibbs-ADAPT-VQE

- Use Renyi divergence-based loss function: $$L(\sigma, \rho) = \log\left(\mathrm{Tr}\left(\sigma^2 \rho^{-1}\right)\right)$$
  - Unbounded → gradients remain large far from solution

Kieferová et al, arXiv:2106.09567



Sherbert et al, arXiv:2408.00218

Still no quantum advantage

What could work out in the near term?

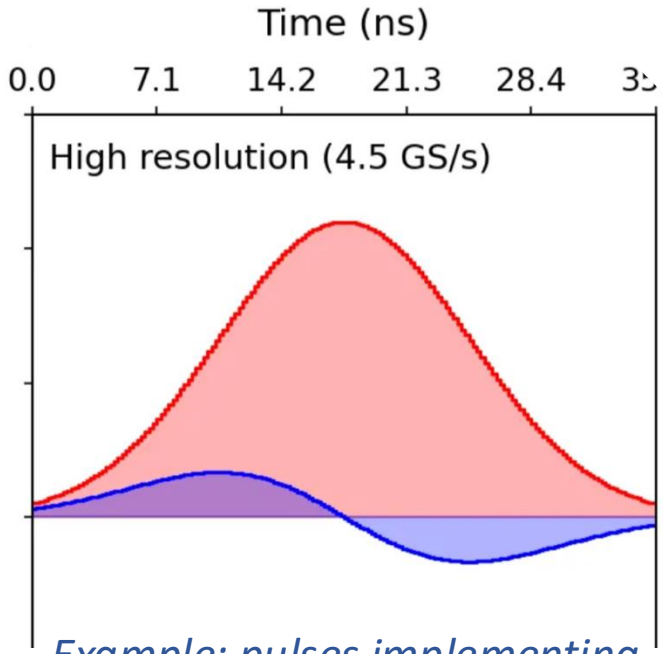
Outline

- Adaptive quantum algorithms (ADAPT-VQA)
  - Background & ADAPT-VQE
  - Adaptive Gibbs state preparation

- Control-VQE: optimizing at the pulse level

Optimizing at the pulse level

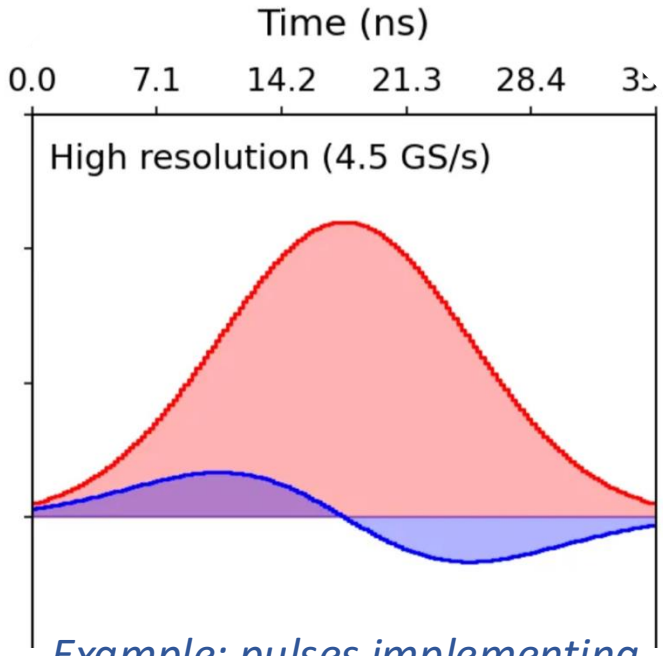
- All gates are made of electromagnetic pulses
- Using gates is a *digitized approach*



Example: pulses implementing IBM single-qubit gates

Optimizing at the pulse level

- All gates are made of electromagnetic pulses
- Using gates is a *digitized approach*



Example: pulses implementing IBM single-qubit gates

Pulse-level optimization:

- Throw out the gates, parameterize pulse directly
- Measure <H>
- Classical optimization → update pulse parameters
- Repeat until convergence

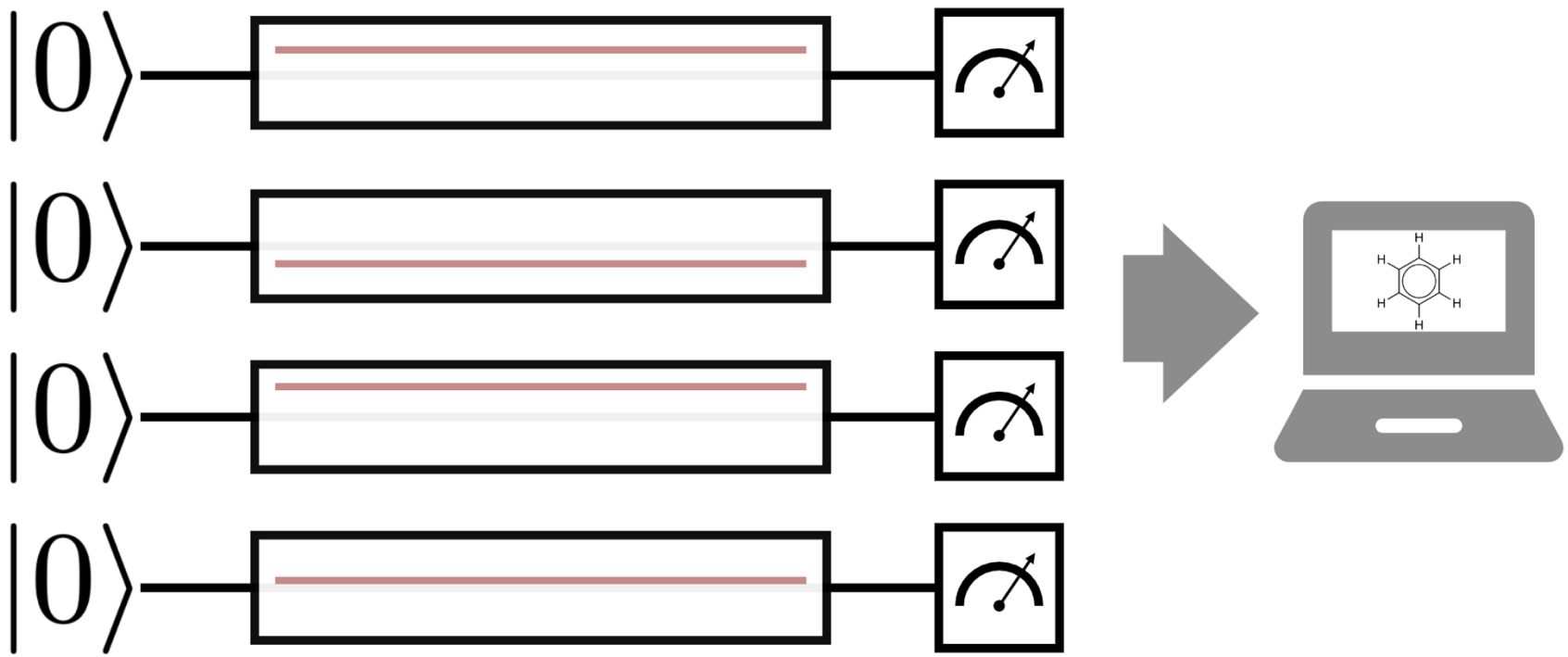
Meitei et al, npj Quantum Information 7, 155 (2021)

Pulse-based parameterization (“ctrl-VQE”)

Gate-based parameterization is a **special case** of pulse parameterization

Lots of freedom in which terms to parameterize, and how to parameterize them

Meitei et al, npj Quantum Information 7, 155 (2021)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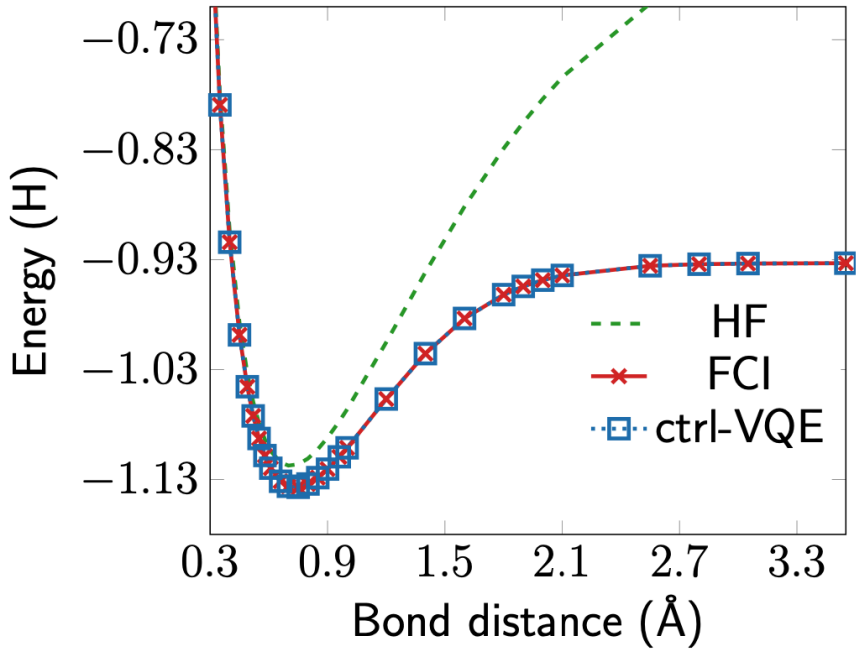
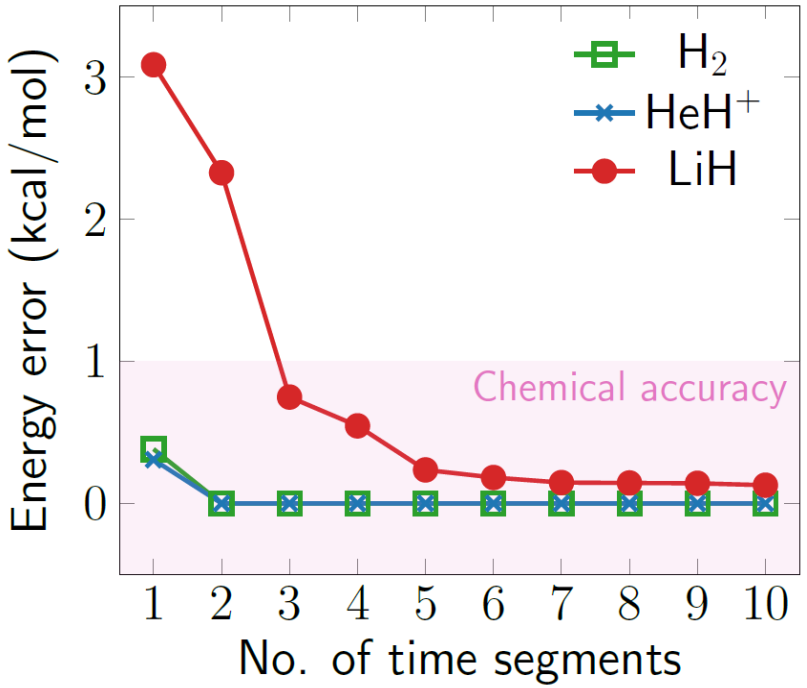
Numerical results

Dissociation curve for H2
(Indistinguishable from FCI)



Number of segments required for convergence



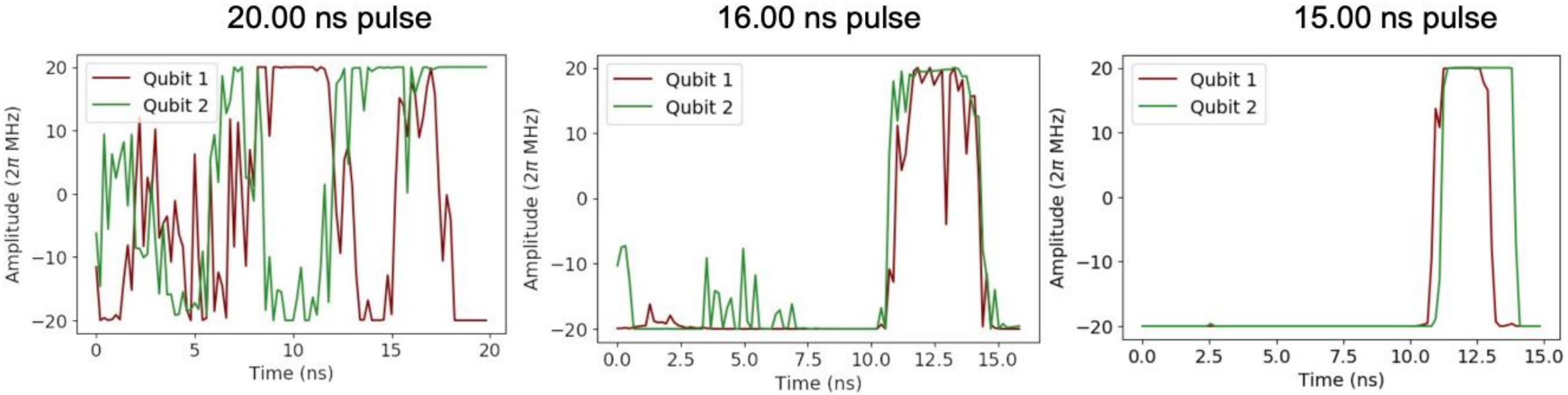
Orders of magnitude improvement:
E.g., for LiH: **80,000ns (gate-based UCCSD) vs. 50ns (ctrl-VQE)**

Meitei et al, npj Quantum Information 7, 155 (2021)

Ctrl-VQE: minimal evolution time

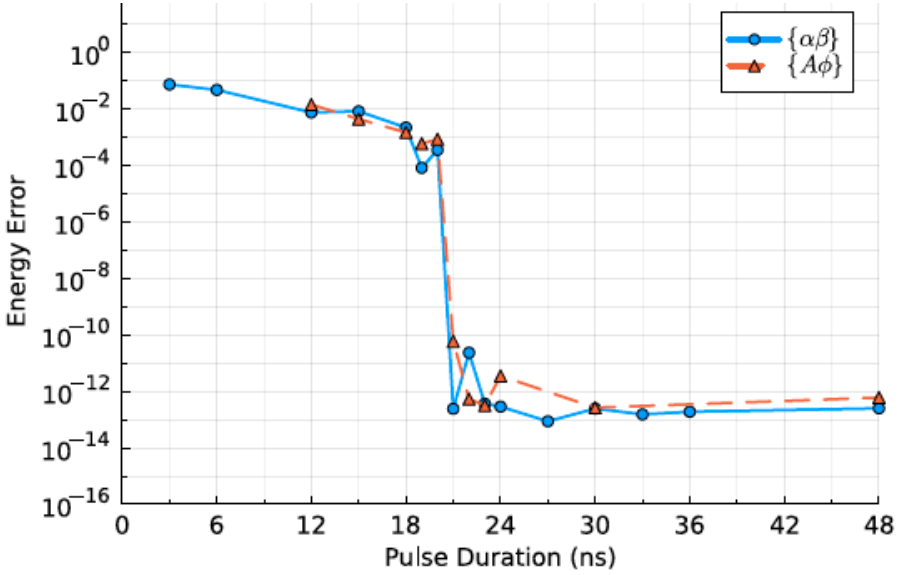
Minimal evolution time (MET): the min time required to transition between two particular quantum states (also referred to as quantum speed limit (QSL))

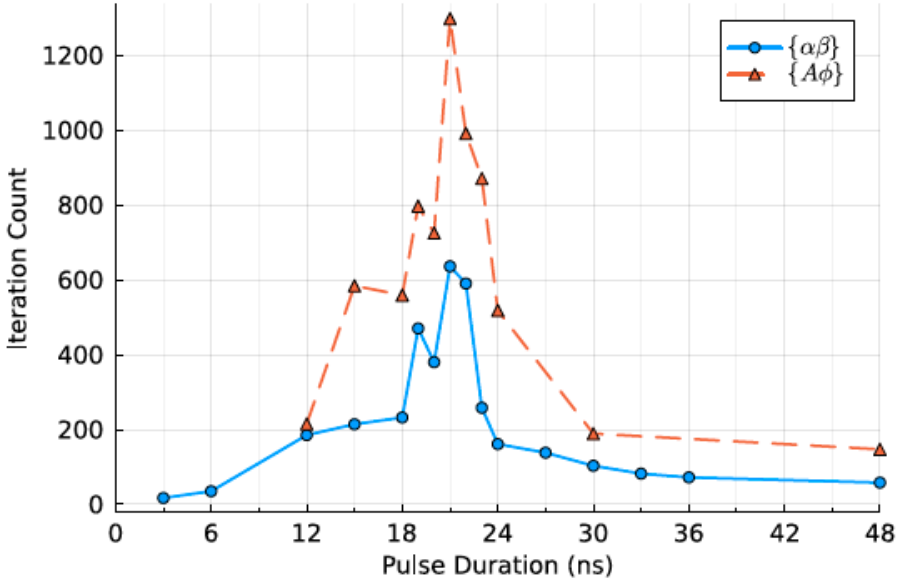
- Below a certain evolution time there is no solution
- Shortening the total pulse time leads to ‘bang-bang’ control (Pontryagin principle)



Asthana, Liu, et al,
Phys. Rev. Applied **19**, 064071 (2023)

Ctrl-VQE: parameterization and optimizability

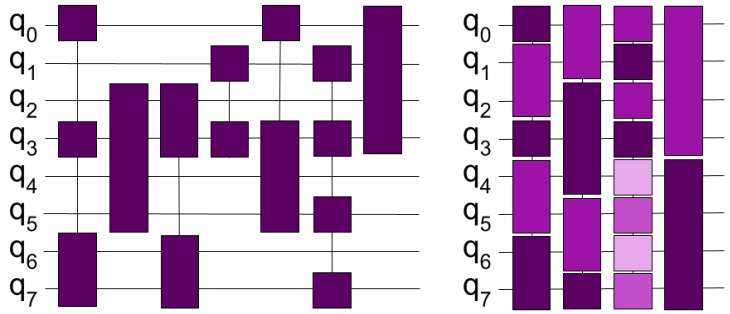


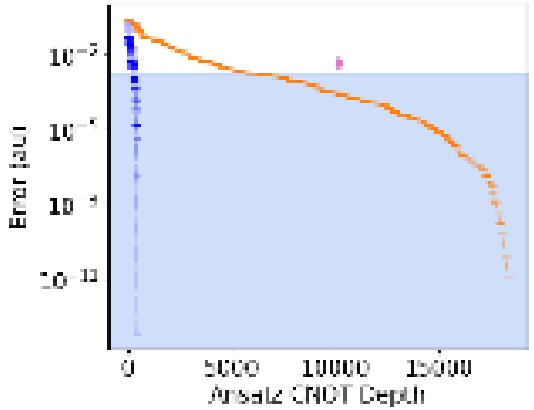


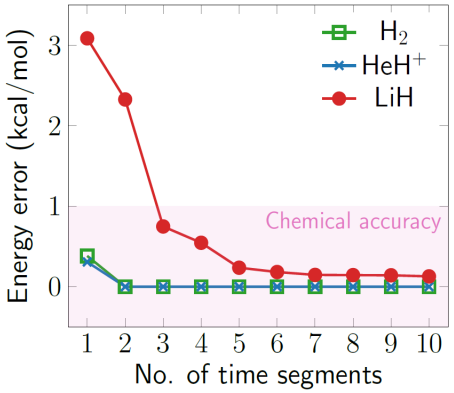
Sherbert, Amer, et al, arXiv:2405.15166

Summary

- ADAPT-VQE
- Algorithmic improvements since 2019
  - TETRIS-ADAPT-VQE (2022)
  - Efficient measurement of gradients (2023)
  - CEO pool (2024)
  - Hessian recycling (2024)
- Adaptive Gibbs state preparation
- Ctrl-VQE







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Virginia Tech


Nick Mayhall
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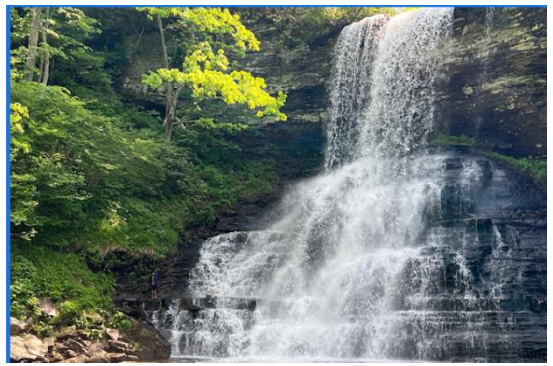
VIRGINIA TECH

Postdoc positions open



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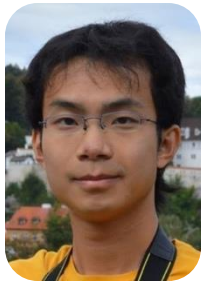

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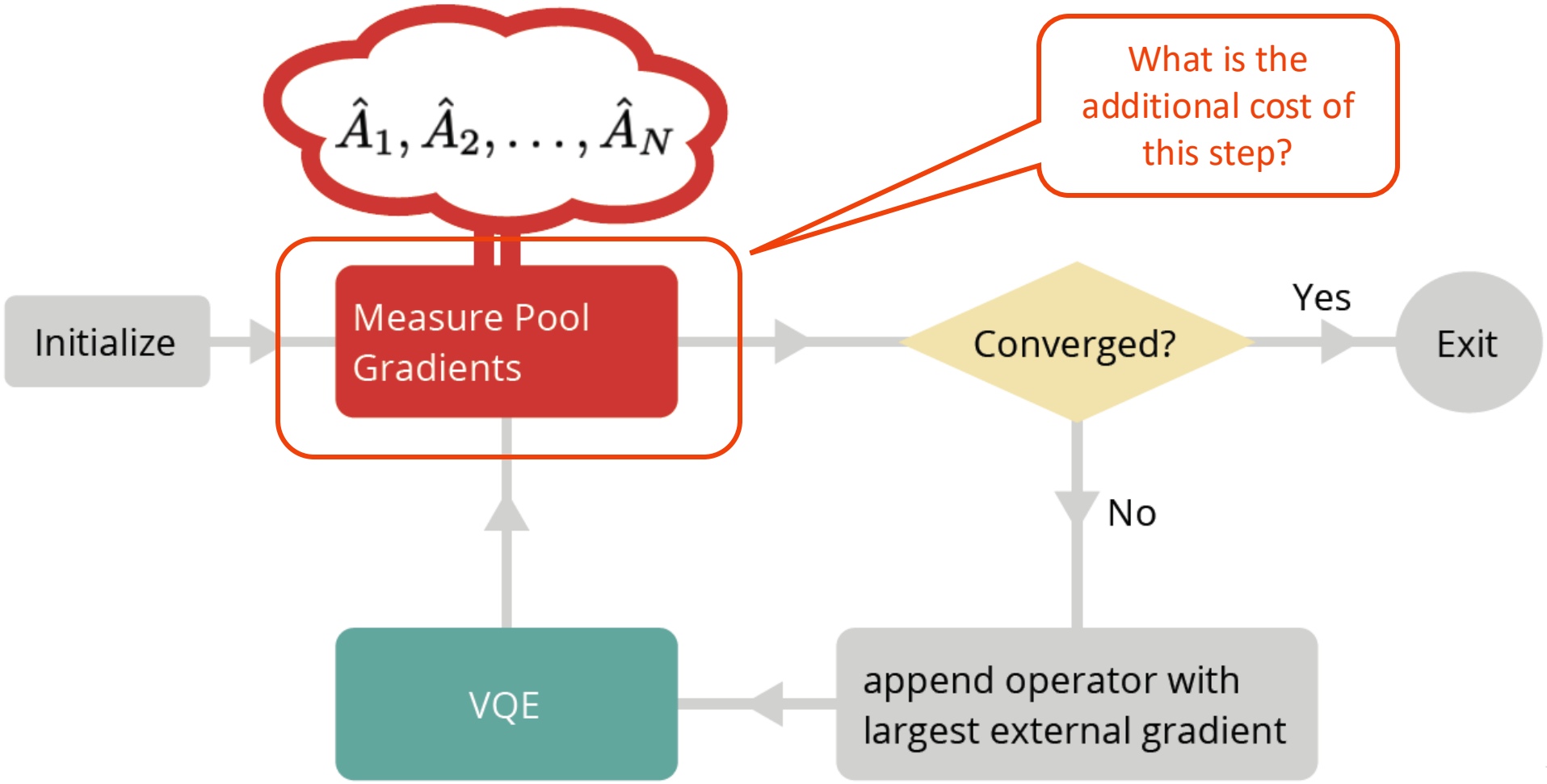
ADAPT-VQE: measurement ‘overhead’



Let’s focus first on the qubit pool (XXXY, etc)

Measuring gradients in ADAPT

$$\left.\frac{\partial E}{\partial \theta_i}\right|_{\theta_i=0} = \left[\frac{\partial}{\partial \theta_i}\left\langle \Psi^{(k)}\right| e^{-\theta_i P_i} H e^{\theta_i P_i} \left|\Psi^{(k)}\right\rangle\right]\Bigg|_{\theta_i=0} = \left\langle \Psi^{(k)}\right| [H, P_i] \left|\Psi^{(k)}\right\rangle$$

Number of terms goes as $O(N^4)$

Size of Pauli pool also goes as $O(N^4)$

- How can we decrease the number of state preparations?

  Commuting observables can be measured simultaneously

- Which grouping heuristic should we use?

  Grouping Hamiltonian terms not ideal

Anastasiou et al, arXiv:2306.03227 (2023)

Measuring gradients in ADAPT—a better approach

For A, B, C Pauli strings:

If $[B, C] = 0$, then $[\,[A, B]\,, [A, C]\,] = 0$

By extension, the commutators of the elements of any mutually commuting set of Pauli strings with any one Pauli string commute

Anastasiou et al, arXiv:2306.03227 (2023)

Measuring gradients in ADAPT—a better approach

What does this mean for operators of the form $iY_iX_jX_kX_l$?

H term	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
					Y	Z	Y	Y	Z	Y	X	Z	X	X	Z	X
S_1	Y	X	X		X											
S_2	Y	X	X			X										
	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
S_3	Y													X	X	X

$O(N^3)$ commutators can be measured simultaneously!

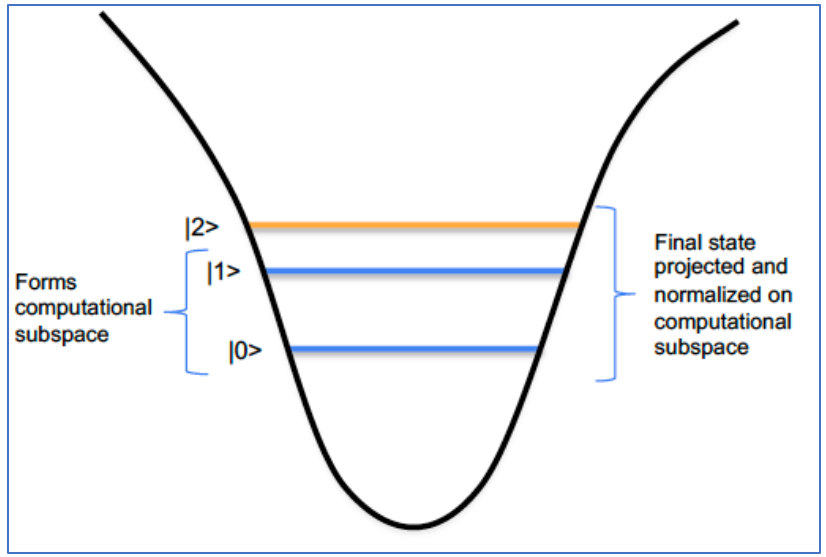
- We can group the commutators of any Hamiltonian term with all qubit operators into $2N$ groups
- Measuring term-by-term of the Hamiltonian means all observables in any given group have the same weight – lower shot-noise
- Measuring the pool gradient is only $\sim N$ times as expensive as a naïve VQE iteration
- QE and CEO pools contain same commuting terms → approach carries over

Anastasiou et al, arXiv:2306.03227 (2023)

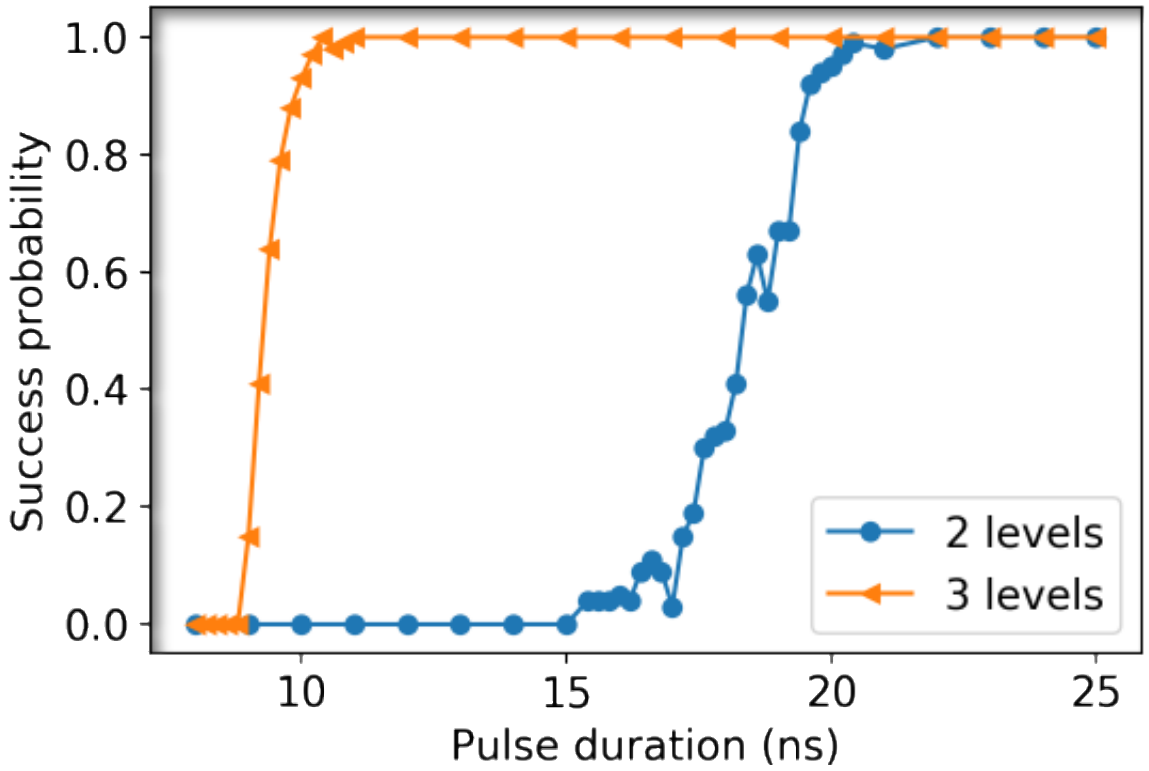
Ctrl-VQE: minimal evolution time

A (possibly surprising) finding:

Leakage to excited states outside qubit space ***speeds up evolution***



Probability to reach exact solution



Simulations for H2 at bond distance 1.5 A

Asthana, Liu, et al,
Phys. Rev. Applied **19**, 064071 (2023)