Subspace-enhanced Variational Quantum Eigensolvers via k-frame optimization

Marco Intini
marco.intini@phd.unipi.it

Collaborator: Giuseppe Clemente

Università di Pisa
Istituto Nazionale di Fisica Nucleare

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Ground state via k-frame

Challenge: Approximate ground states of many-body Hamiltonians (using NISQ devices)

- **Goal**: Study systems in cases of no apparent problem structure

When traditional variational approaches face **limitations**:

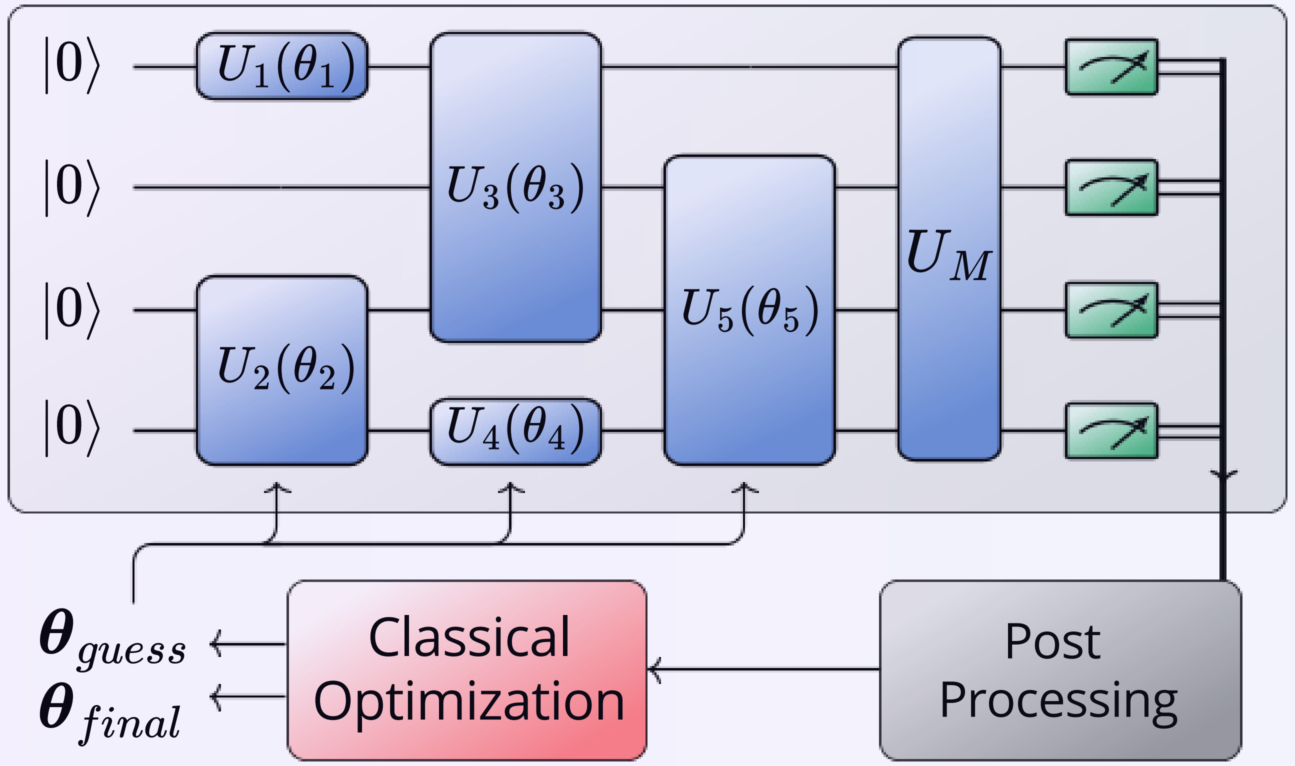
- Minimal exploitable symmetries (e.g. spin glasses)
- Problem-inspired solutions may require excessive resources

K-frame **approach**: Optimize over subspaces instead of single states

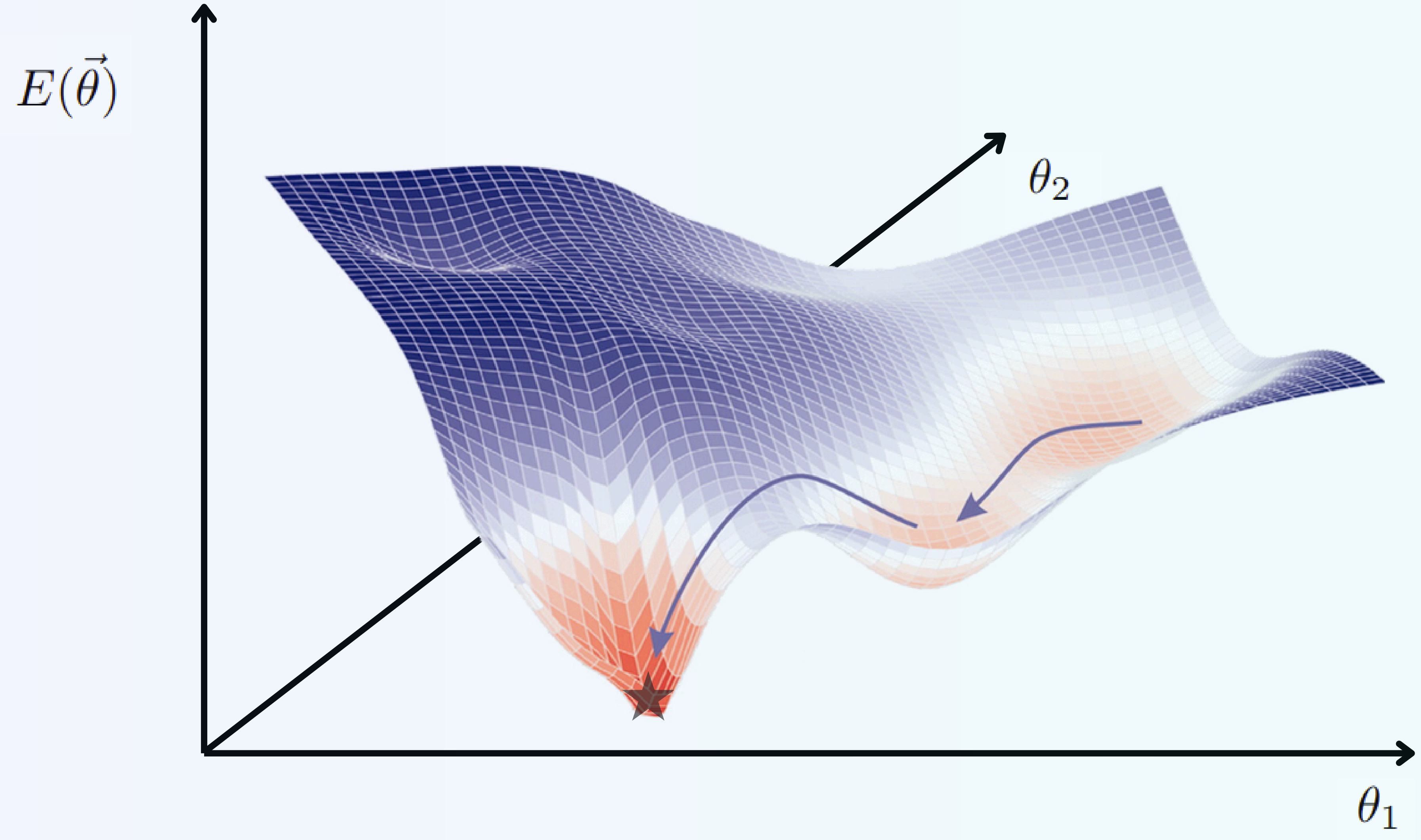
- standard VQE : 1 parametric circuit ⟶ 1 single state
- k-frame: k parametric circuits ⟶ any linear combinations of k states

VQA = Quantum explorer, Classical guide

1. Inizialize state **Q**
2. Apply parametrized unitaries (ansatz) **Q**
3. Evaluate expectation energy **Q**
4. Optimize $\theta \to \theta + \delta\theta$ **C**



VQAs scheme [Bittel et al., PRL (2021)]



Variational Quantum Eigensolvers (VQE)

Minimize $E(\boldsymbol{\theta}) = \langle\psi(\boldsymbol{\theta})|H|\psi(\boldsymbol{\theta})\rangle$ with $|\psi(\boldsymbol{\theta})\rangle = \prod_i U_i(\theta_i)|\mathbf{0}\rangle$

[0] Peruzzo et al. (2014). A variational eigenvalue solver on a photonic quantum processor. Nature Communications, 5(1), 4213.

Ansatz Choices

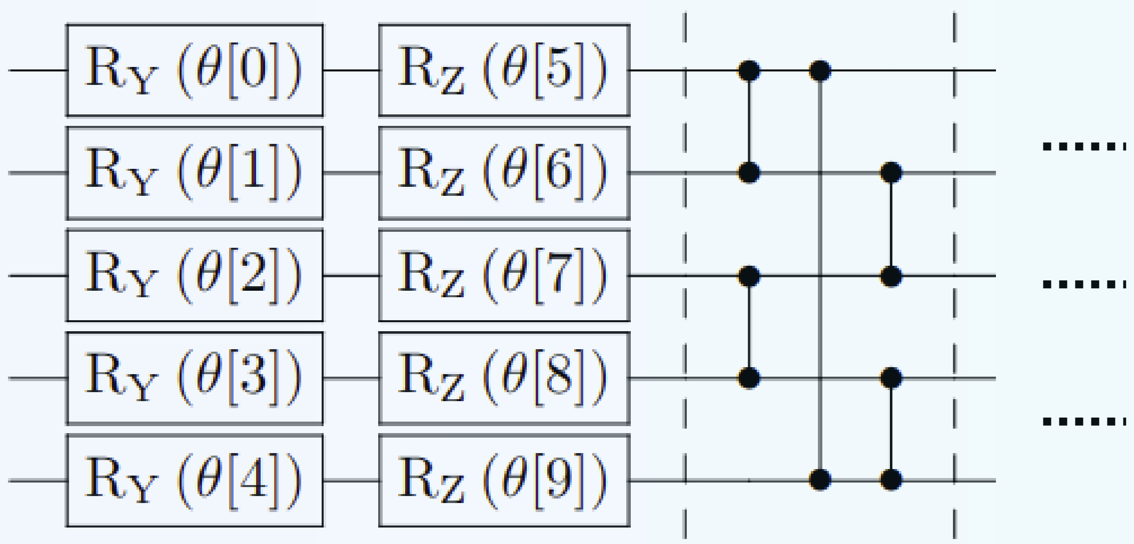
PROBLEM INSPIRED

$$|\psi(\boldsymbol{\theta})\rangle = \prod_{m=1}^{R} e^{-i\theta_{m,M}H_M} \cdots e^{-i\theta_{m,1}H_1} |\psi_0\rangle$$

Hamiltonian is a linear combination of these generators

- These are symmetry-preserving ansätze known as Hamiltonian Variational Ansatz
- Low-depth only for specific problems

AGNOSTIC

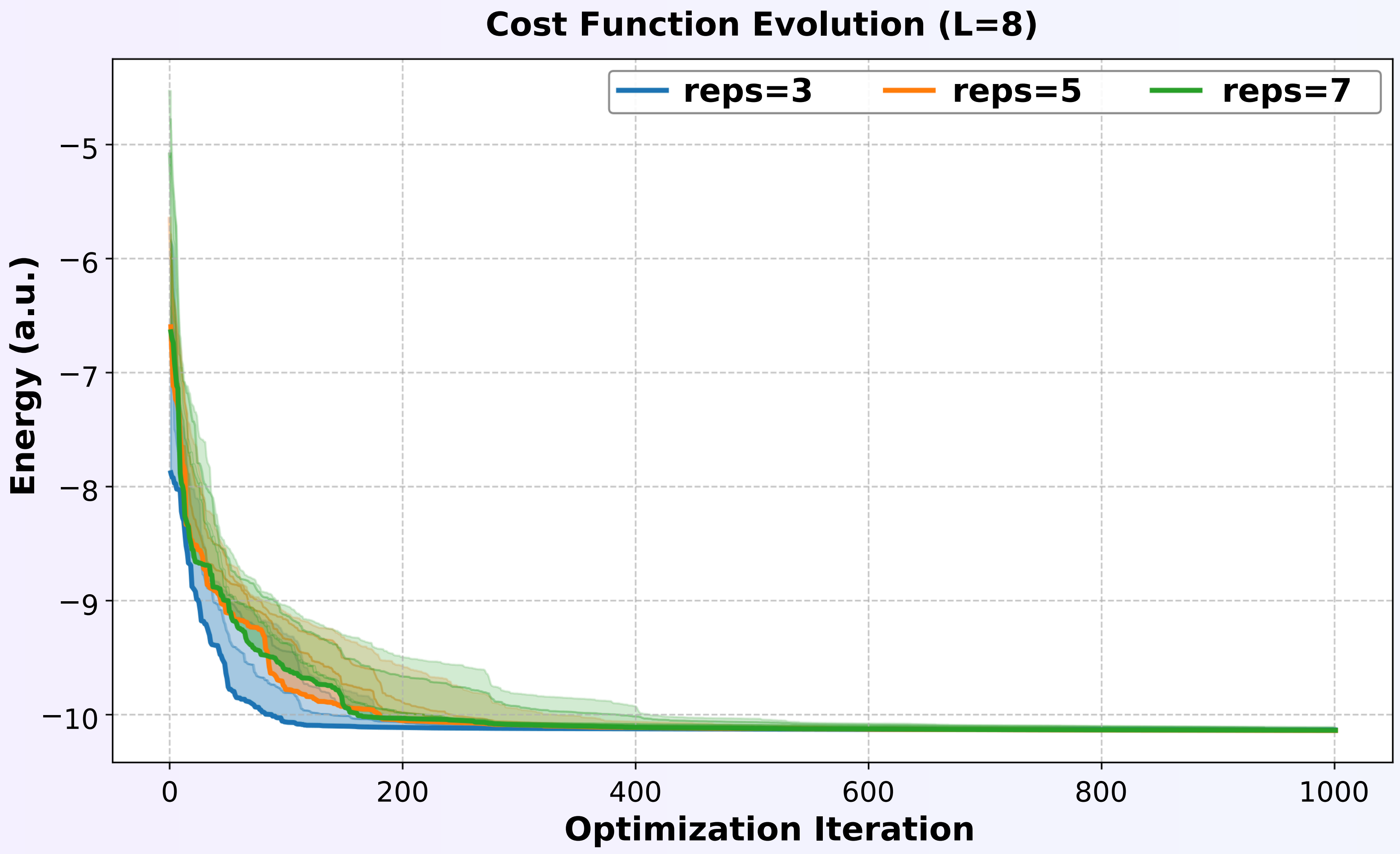


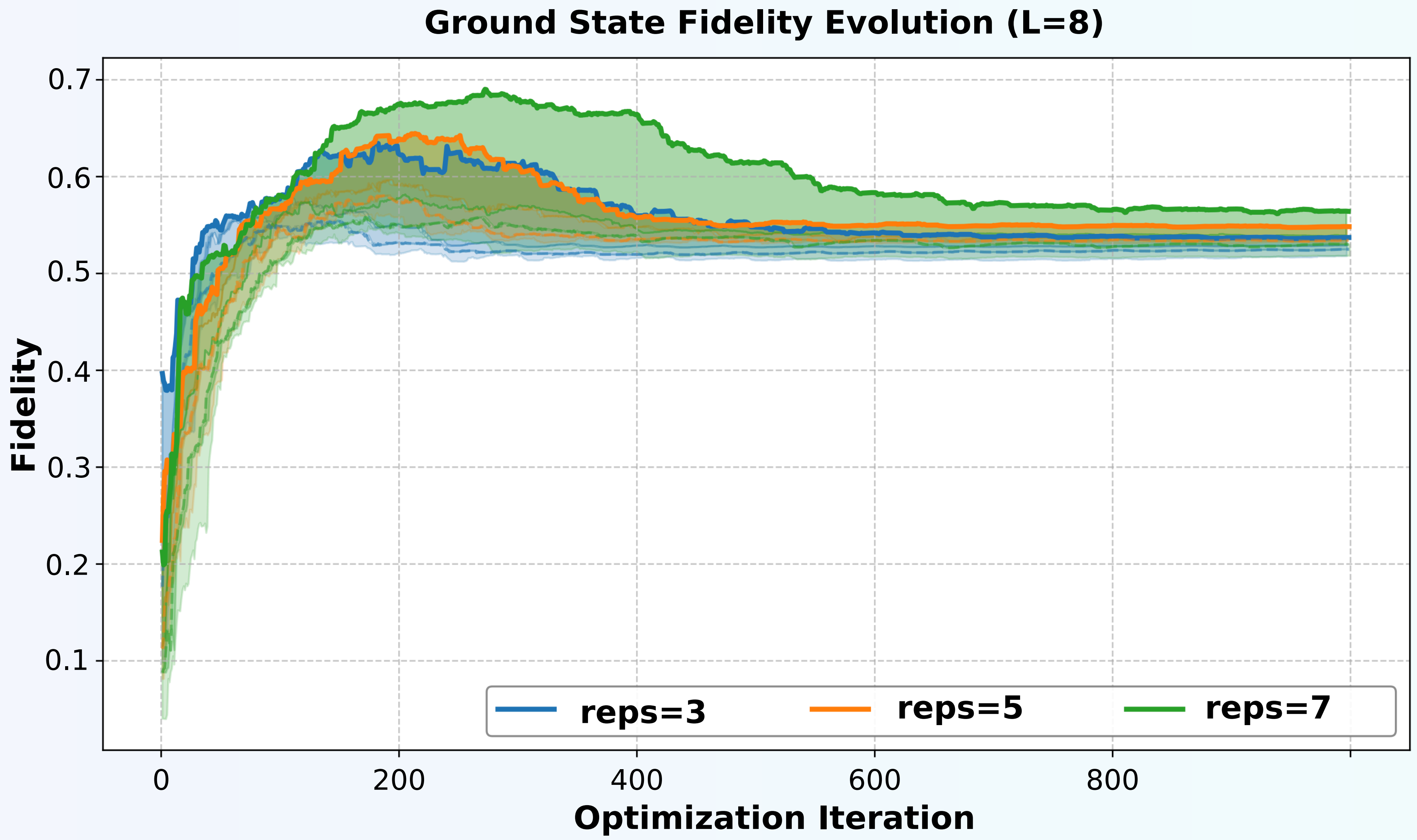
Repeated R times

- Characterized by expressibility and entanglement
- Typically requires more parameters

1D Ising Chain $H = -J\sum_{j=1}^{N} X_j X_{j+1} - h\sum_{j=1}^{N} Z_j = H_1 + H_2$

VQE 1D Ising Chain PBC (at criticality)

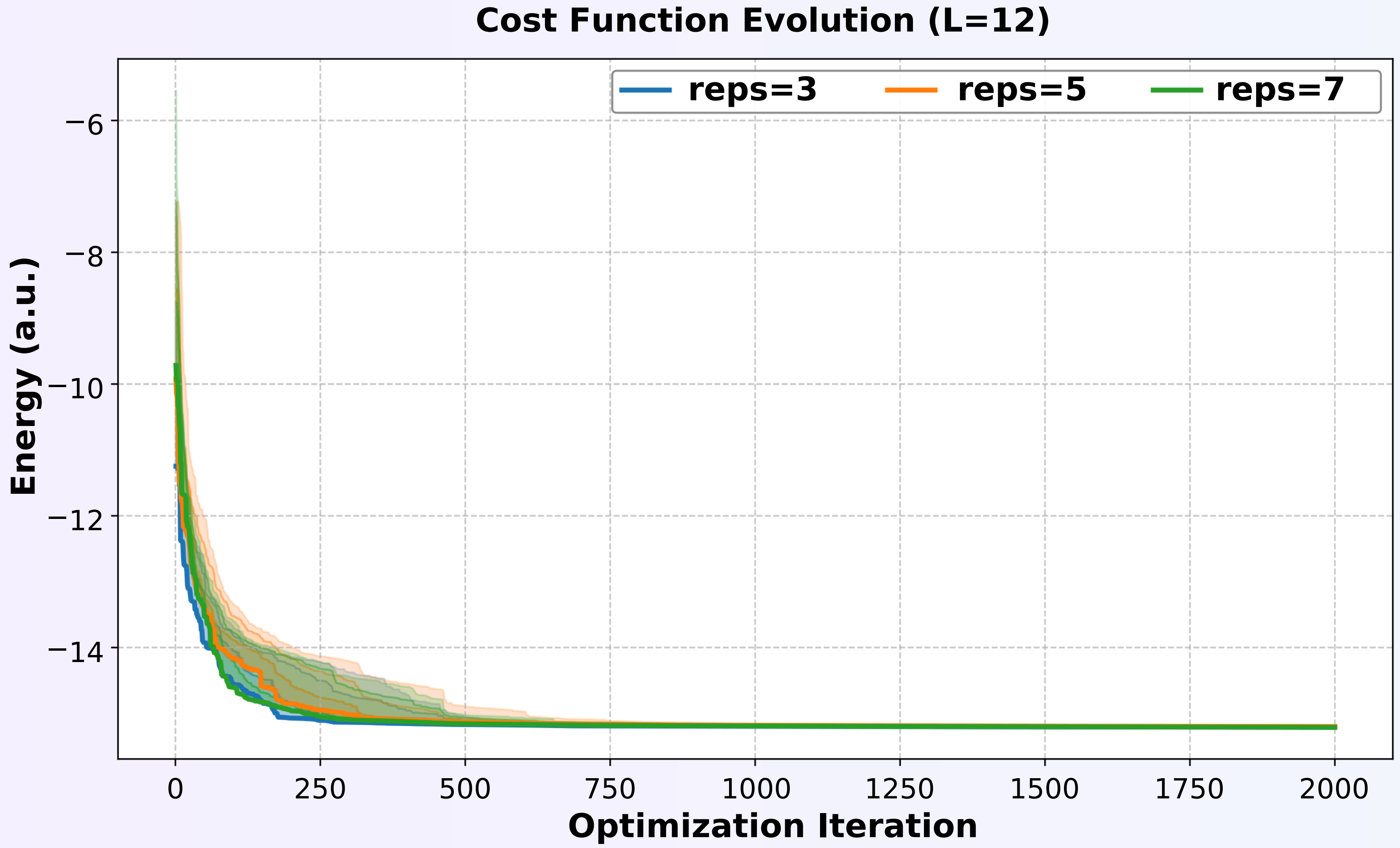


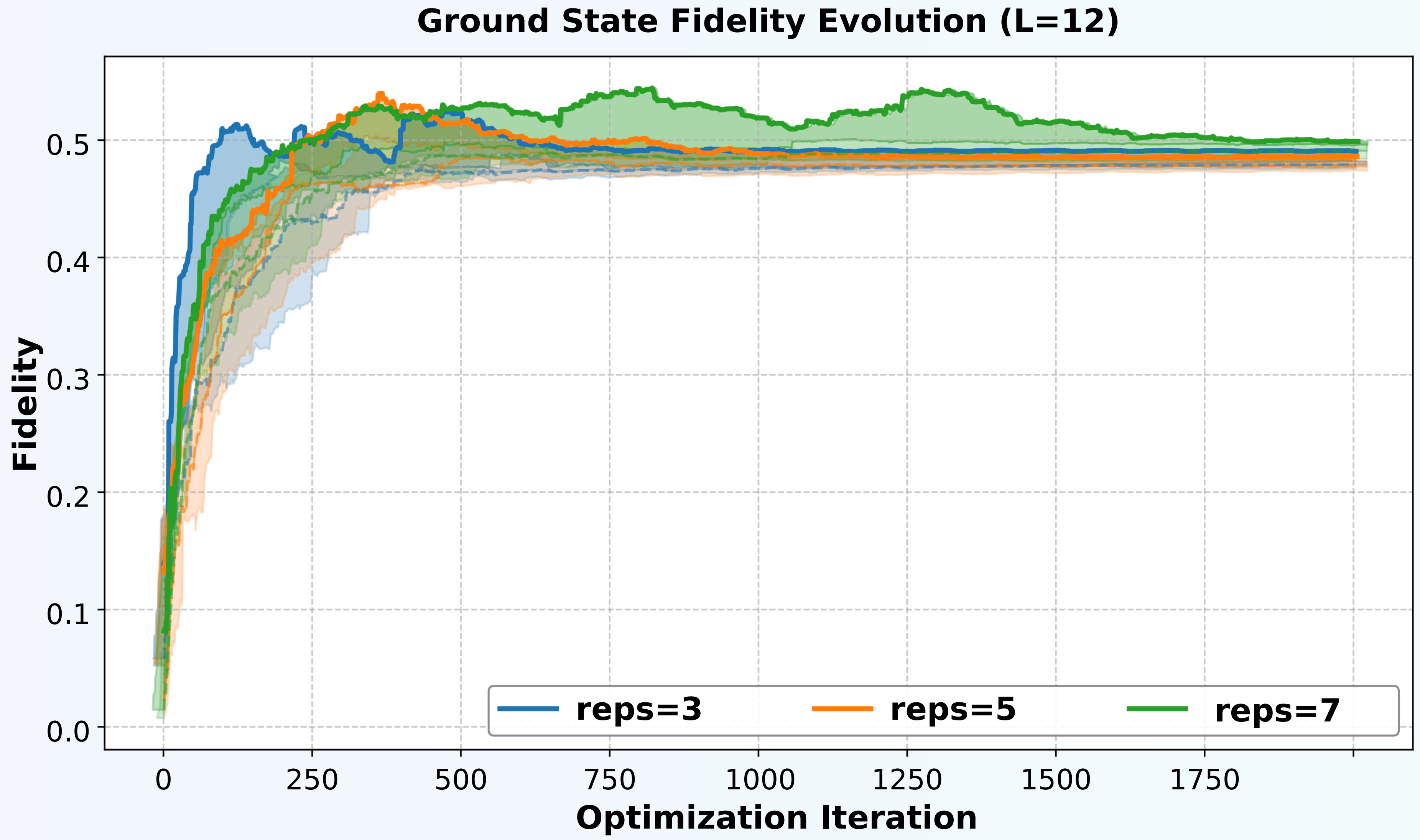


- At convergence, $|\langle\phi_{GS}^{EX}|\psi(\theta)\rangle|^2 \sim 0.55$ even using up to 7 layers
- Adding parameters does not improve performance, optimization slows after $\sim\, 400$ iterations

10 x independent runs for any set of reps

VQE 1D Ising Chain PBC - L=12





- Optimization requires more iterations for larger systems
- Problem becomes more challenging as quantum resources scale

Need for improvements to the standard VQE approach

Extentions of VQE: excited states

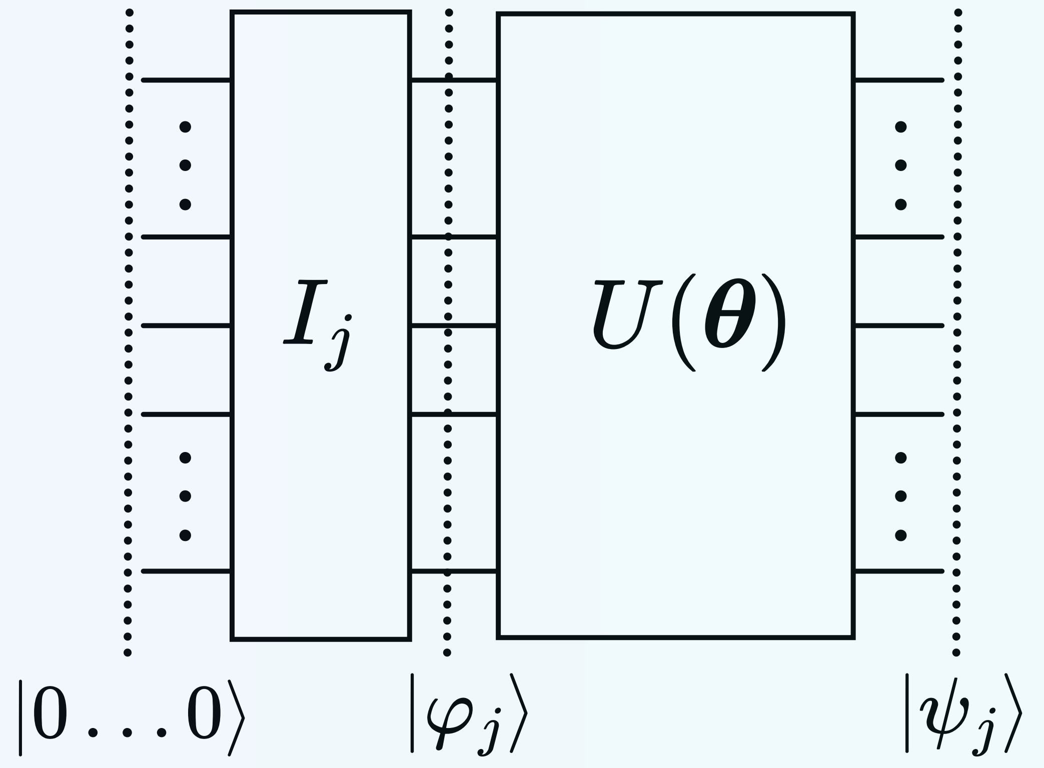
Subspace-search VQE (SSVQE) [1]:

1. Construct ansatz $U(\theta)$, choose input states orthogonal with each other $\langle\varphi_i|\varphi_j\rangle = \delta_{ij}$,e.g. $|\varphi_j\rangle = I_j|\mathbf{0}\rangle$
2. Minimize $\mathcal{L}_w(\boldsymbol{\theta}) = \sum_{j=1}^{k} w_j \langle\varphi_j|U^\dagger(\theta) H U(\theta)|\varphi_j\rangle$ with $\omega_i < \omega_j$ if $i < j$

Possible to measure transition amplitude of an operator A: $\langle\psi_i|A|\psi_j\rangle$

MC-VQE [2]:

- Same as SS-VQE with $w_k = 1 \ \forall k$
- After minimization procedures measure $\langle\psi_i|H|\psi_j\rangle$
- Diagonalize Hamiltonian in this subspace



[1] Nakanishi, Mitarai & Fujii (2019). Subspace-search variational quantum eigensolver for excited states. PRR, 1(3), 033062.
[2] Parrish et al. (2019). Quantum Computation of Electronic Transitions Using a Variational Quantum Eigensolver. PRL, 122(23), 230401.

Extentions of VQE: excited states (con't)

Variational Quantum Deflation (VQD) [3]: (AKA k-VQE + deflation terms)

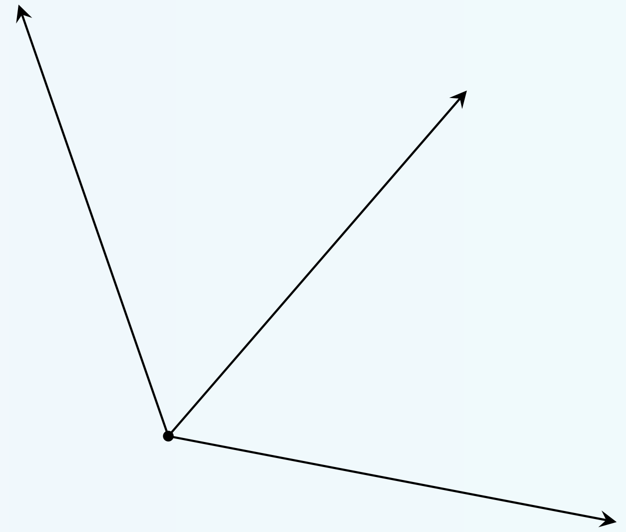
1. Use VQE to find ground state $|\psi(\theta_1)\rangle$
2. Find 1-st excited ansatz state by mimizing $\mathcal{L}(\theta_2) = \langle\psi(\theta_2)|H|\psi(\theta_2)\rangle + \beta_1 |\langle\psi(\theta_2)|\psi(\theta_1)\rangle|^2$
3. Iteratively find k-1 excited ansatz state by minimizing $\mathcal{L}(\theta_k) = \langle\psi(\theta_k)|H|\psi(\theta_k)\rangle + \sum_{i=0}^{k-1} \beta_i |\langle\psi(\theta_k)|\psi(\theta_i)\rangle|^2$

We use parallel & uniformly weighted version:

$$\mathcal{L}(\theta_1, \ldots, \theta_k) = \sum_{i=1}^{k} \langle\psi(\theta_i)|H|\psi(\theta_i)\rangle + \beta \sum_{i\neq j} |\langle\psi(\theta_j)|\psi(\theta_i)\rangle|^2$$

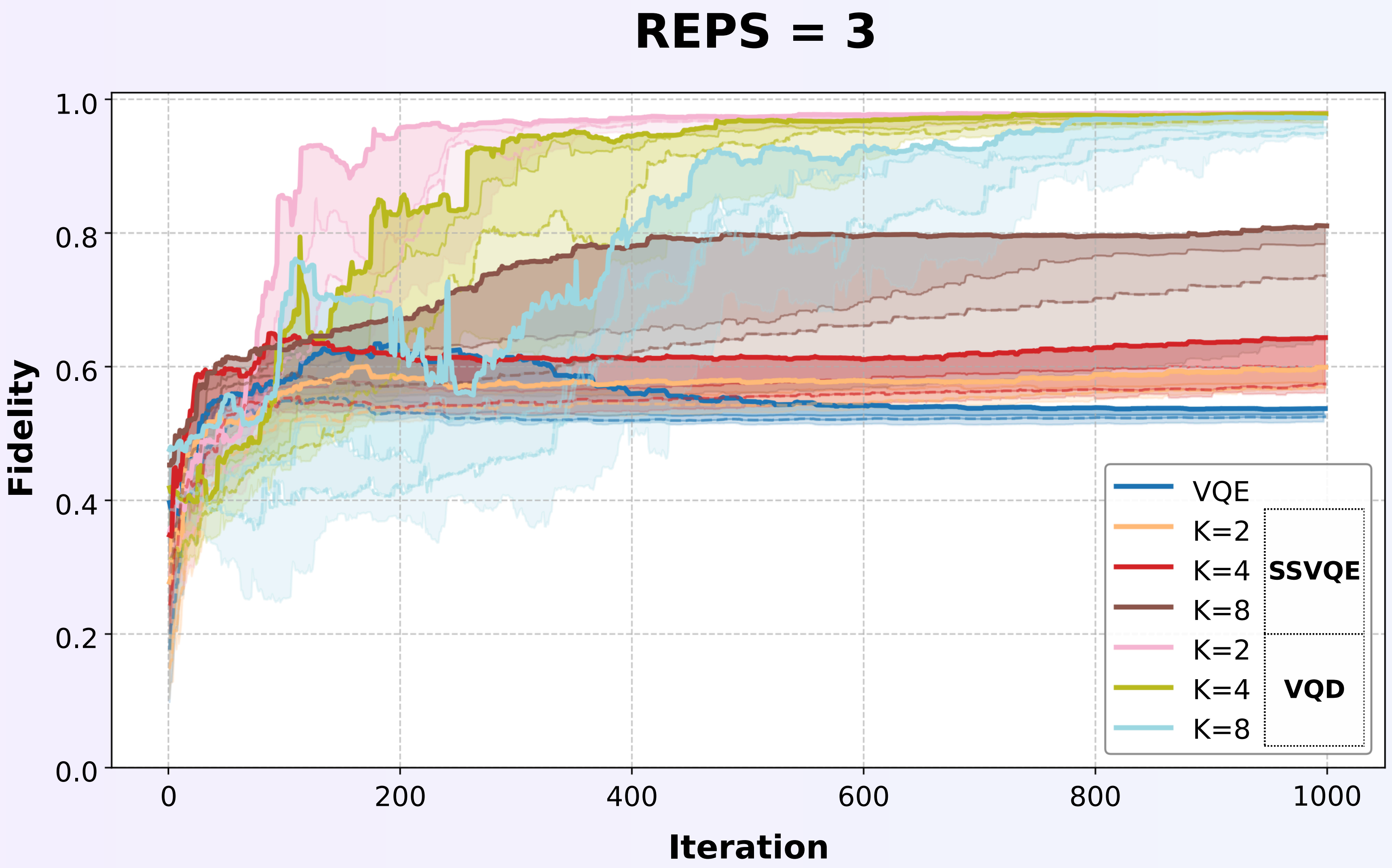
- After convergence measure $\langle\psi_i|H|\psi_j\rangle$
- Diagonalize k x k effective Hamiltonian

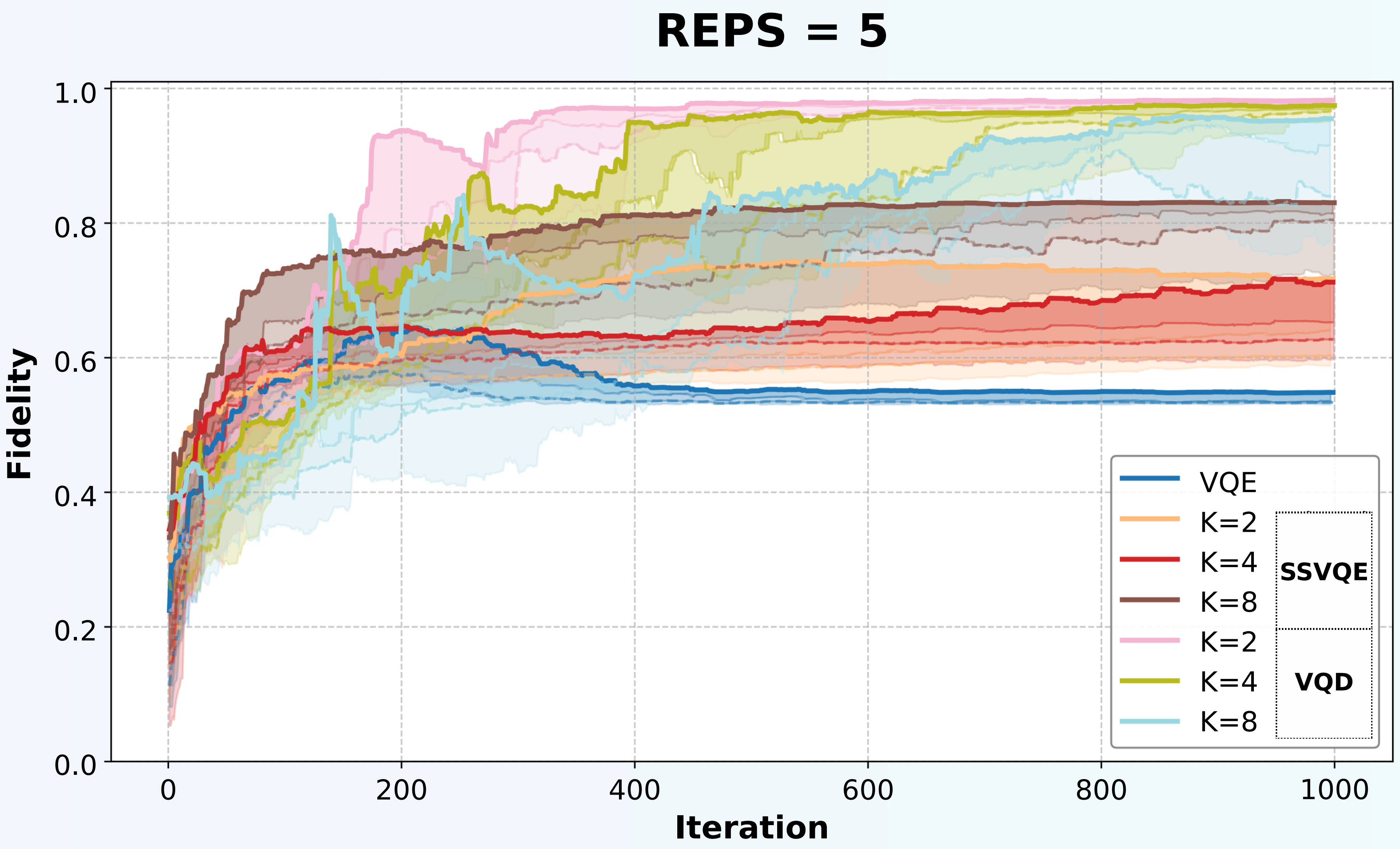
3-frame



[3] Higgott, Wang & Brierley (2019). Variational Quantum Computation of Excited States. Quantum, 3, 156.

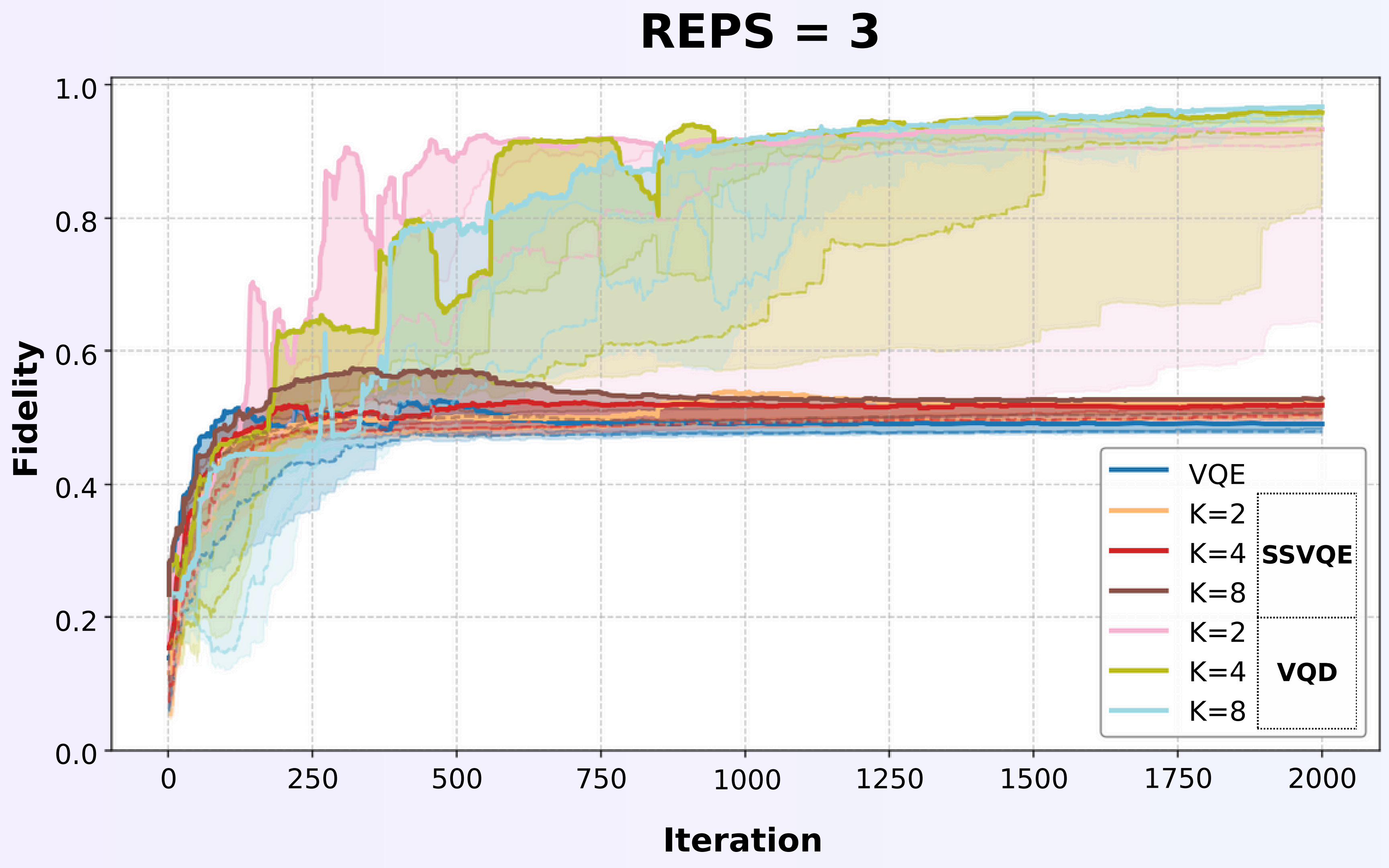
GS Fidelity Evolution L=8

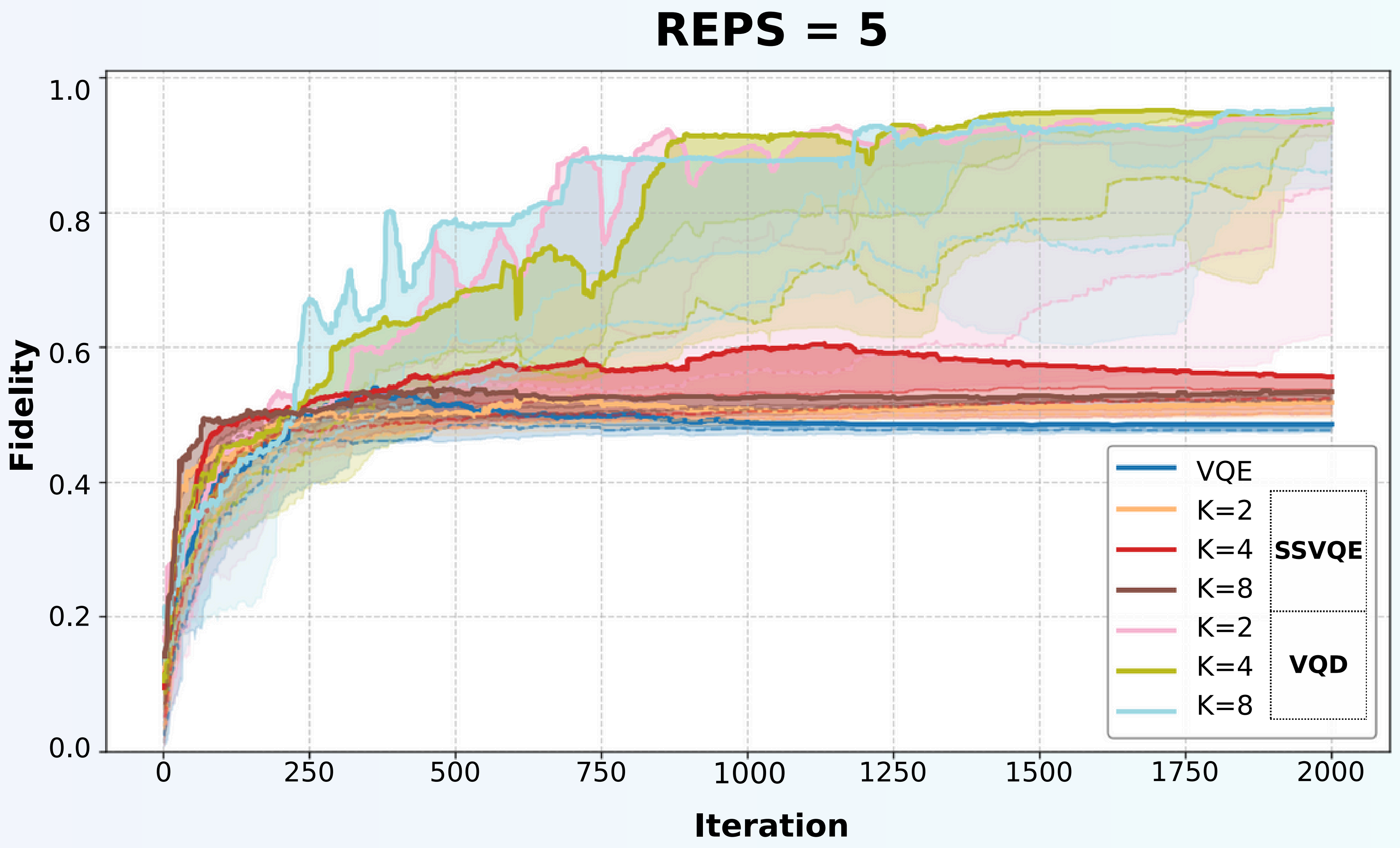




- K-frame approaches (both SSVQE and VQD) significantly outperform standard VQE
- VQD achieves ~95% fidelity vs ~80% for SSVQE and ~55% for VQE
- Efficient convergence with just 3 reps (shallow circuits)

GS Fidelity Evolution L=12





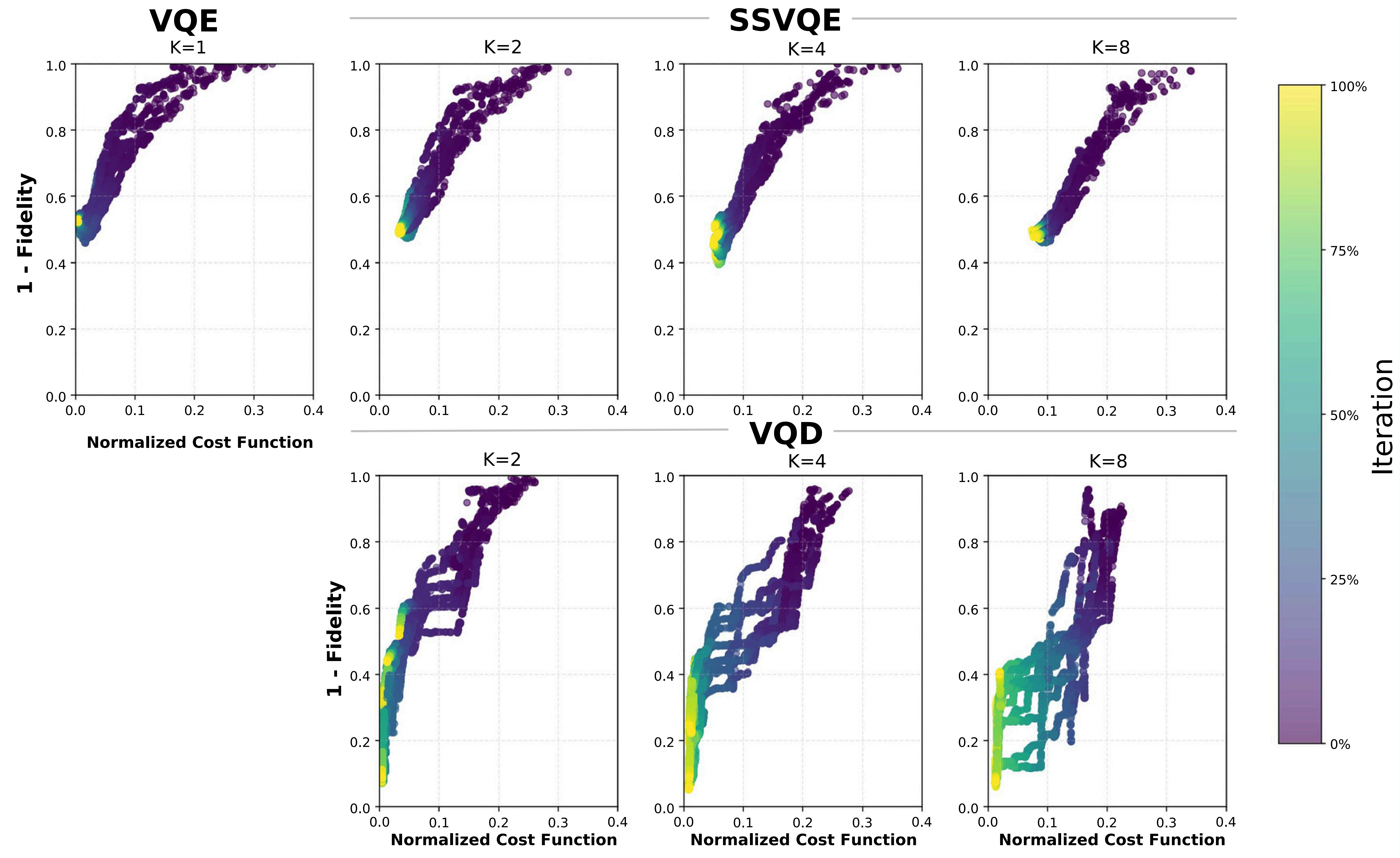
- VQD maintains superior performance (~95% fidelity) even at L=12
- Performance gap between VQD and SSVQE widens with system size

Cost-Infidelity Correlation (L=12, reps=5)

SSVQE exhibits weaker cost-fidelity correlation compared to VQD

Steeper cost-fidelity correlation in VQD, more efficient convergence

VQD shows **two** distinct optimization phases (visible as "steps")



the trend seems preserved at different sizes and parameters

Conclusions and outlook

KEY FINDINGS

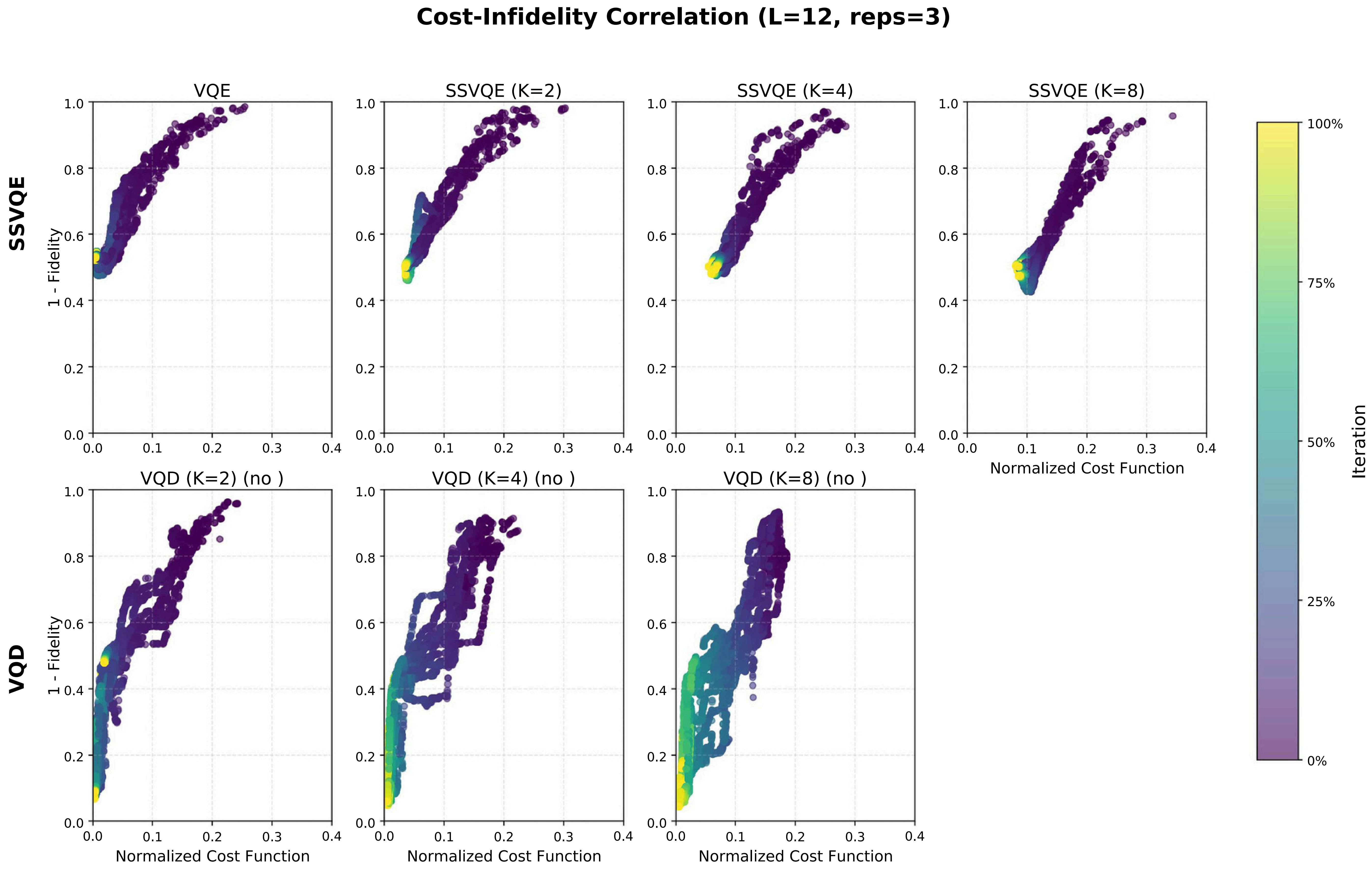
- K-frame outperform standard VQE (95% vs 55% fidelity) for the 1D Ising model
- VQD demonstrates superior convergence properties compared to SSVQE
- VQD shows better higher sensitivity of fidelity to cost improvements

FUTURE DIRECTIONS

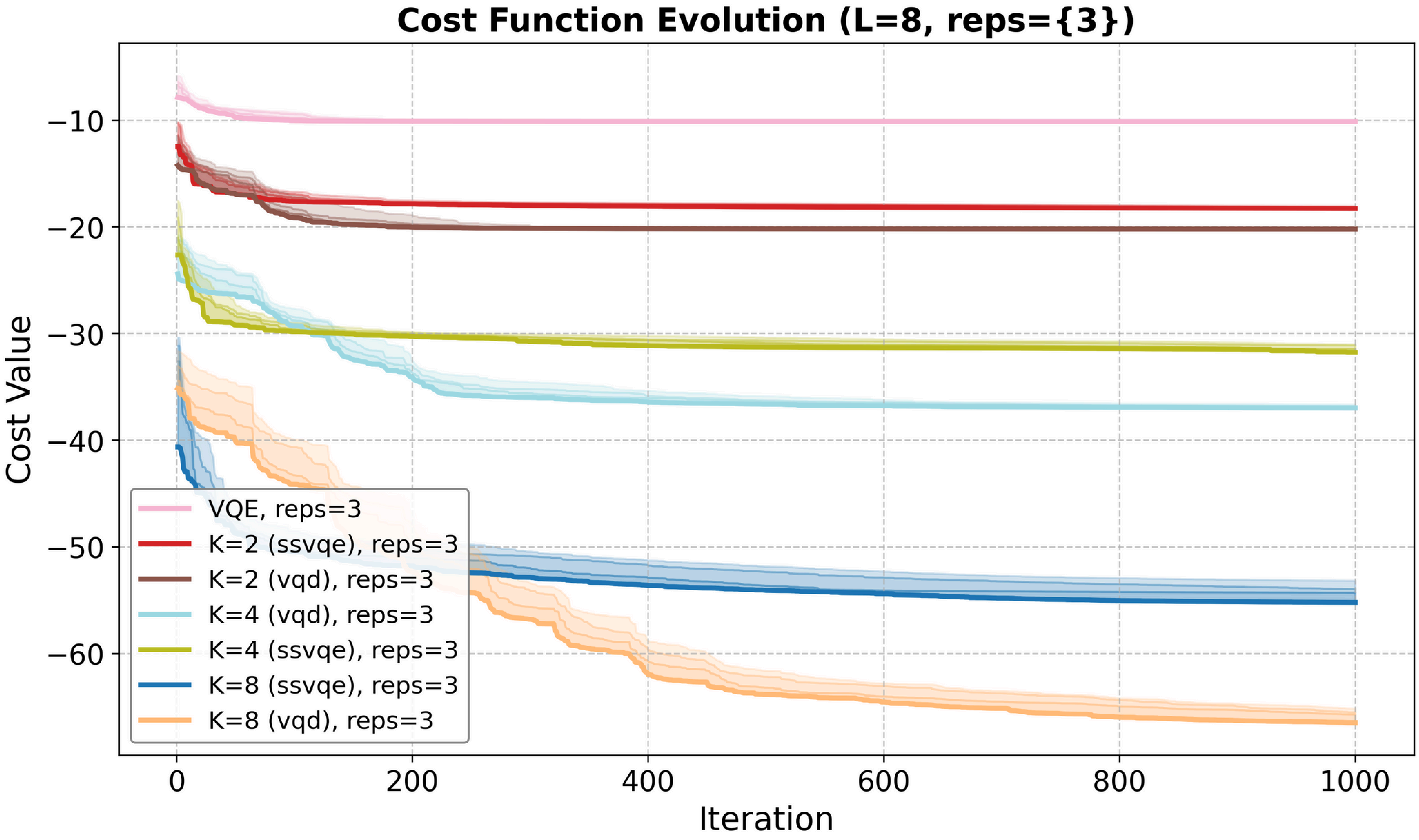
- Extend to larger system sizes (L>12, D=2) to investigate scalability limits
- Study expressibility metrics to quantify representation advantages of k-frame approaches
- Apply to more complex Hamiltonians without clear symmetries
  (e.g. spin glasses, disordered systems)

Thank you for the attention!

Backup



Cost-Infidelity Correlation (L=12, reps=3)
SSVQE
VQD
VQE
SSVQE (K=2)
SSVQE (K=4)
SSVQE (K=8)
VQD (K=2) (no)
VQD (K=4) (no)
VQD (K=8) (no)
1 - Fidelity
Normalized Cost Function
Iteration
100%
75%
50%
25%
0%


Cost Function Evolution (L=8, reps={3})
Cost Value
Iteration
−10
−20
−30
−40
−50
−60
0
200
400
600
800
1000
VQE, reps=3
K=2 (ssvqe), reps=3
K=2 (vqd), reps=3
K=4 (vqd), reps=3
K=4 (ssvqe), reps=3
K=8 (ssvqe), reps=3
K=8 (vqd), reps=3