# Enhancing Convergence in Variational Quantum Eigensolver Using CoolMomentum

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## 1. Introduction: Gate-Based Quantum Computer

### ◆ Noisy Intermediate-Scale Quantum Device

J. Preskill, Quantum 2 (2018) 79.

✓ Resent Quantum Processing Unit (QPU) called NISQ Device.
✓ Now, NISQ Device with Hundreds of Qubits is Available.

IBM Heron (133 Qubits)


https://newsroom.ibm.com/

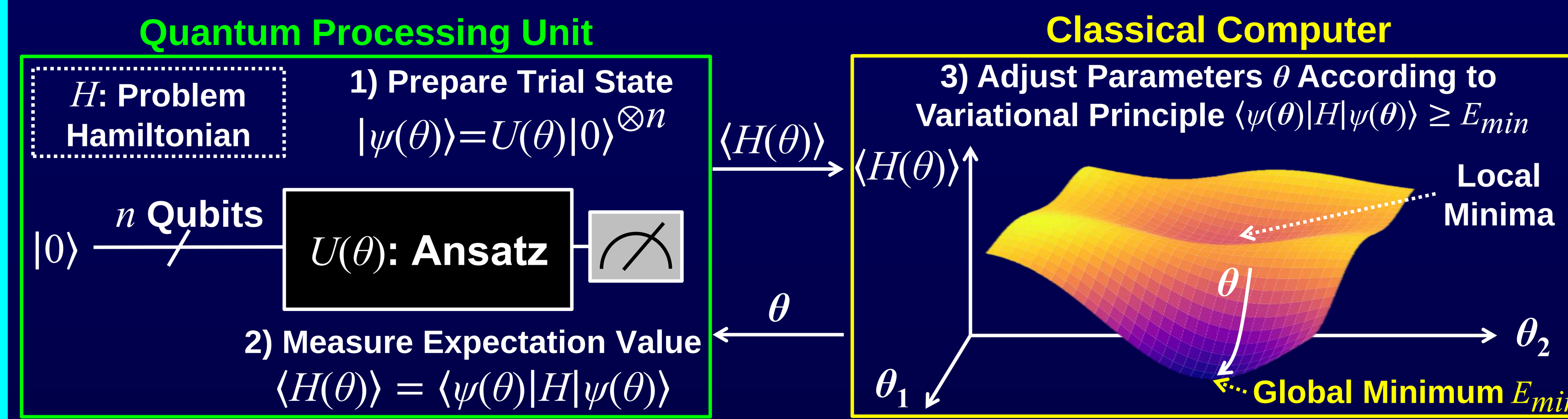
- Limited Number of Qubits
- Too Few Physical Qubits to Implement Robust Error Correction Schemes.
- Gate Errors and Decoherence Restrict Number of Sequential Gate Operations

One of Promising Approaches Leveraging NISQ is Quantum-Classical Hybrid Algorithm.

### ◆ Variational Quantum Eigensolver (VQE)

A. Peruzzo, et al., Nat. Commun. 5 (2014) 4213.

✓ Quantum-Classical Hybrid Algorithm Used to Find Ground State Energy of a Hamiltonian.
✓ VQE can be Used Both for Classical Optimization Problems as well as for Fermionic Hamiltonians.

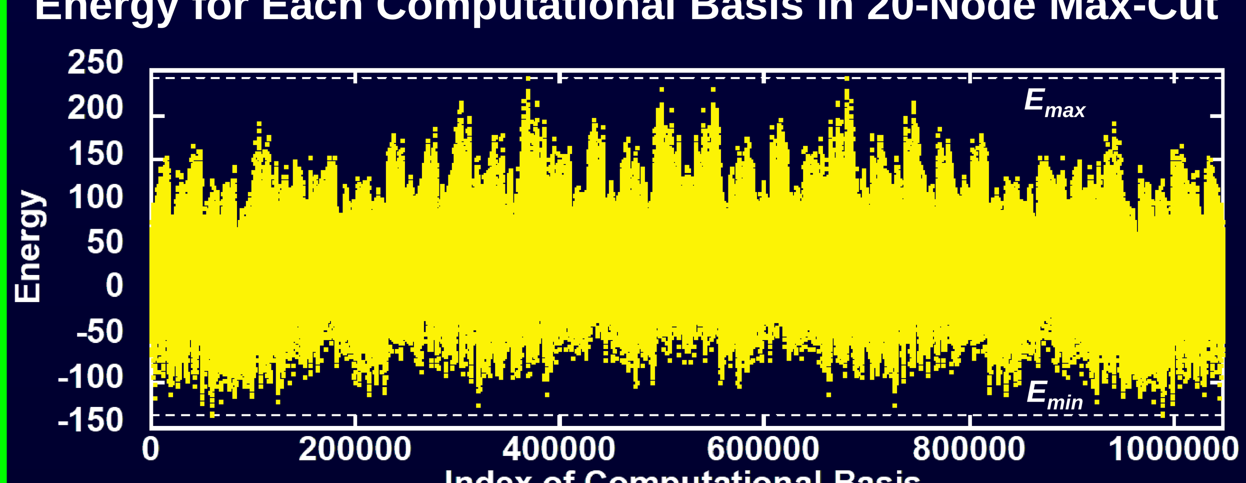



## 2. Challenges in VQE and Our Approach in This Study

### ◆ Classical Optimization Problem

Classical Optimization in VQE is Shown to be NP-Hard.
L. Bittel and M. Kliesch, Phys. Rev. Lett. 127 (2021) 120502.
→Finding Optimal Solution to Problem is Intractable.

Energy for Each Computational Basis in 20-Node Max-Cut



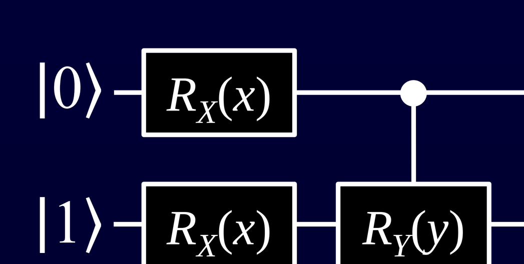

✓ Out of $2^{20}$ Computational Bases, Most are Local Solutions, with Only a Few Being Optimal Solutions.

Problem: Depending on Initial Values of Parameters, There is Possibility of Getting Trapped in Local Minima.

### ◆ Utilizing CoolMomentum Method to Achieve Lower Energy States.

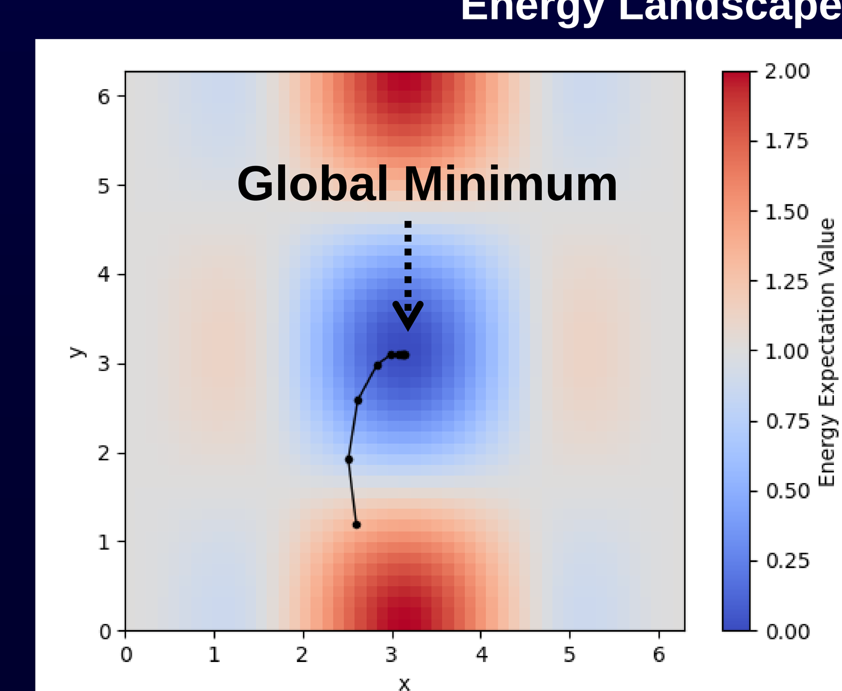
**CoolMomentum:** An Optimizer that Combines Langevin dynamics with Simulated Annealing.
O. Borysenko and M. Byshkin, Sci Rep. 11 (2021) 10705.

Ansatz and Hamiltonian of Toy Model
S. McArdle, et al., Npj Quantum Inf. 5 (2019) 75.

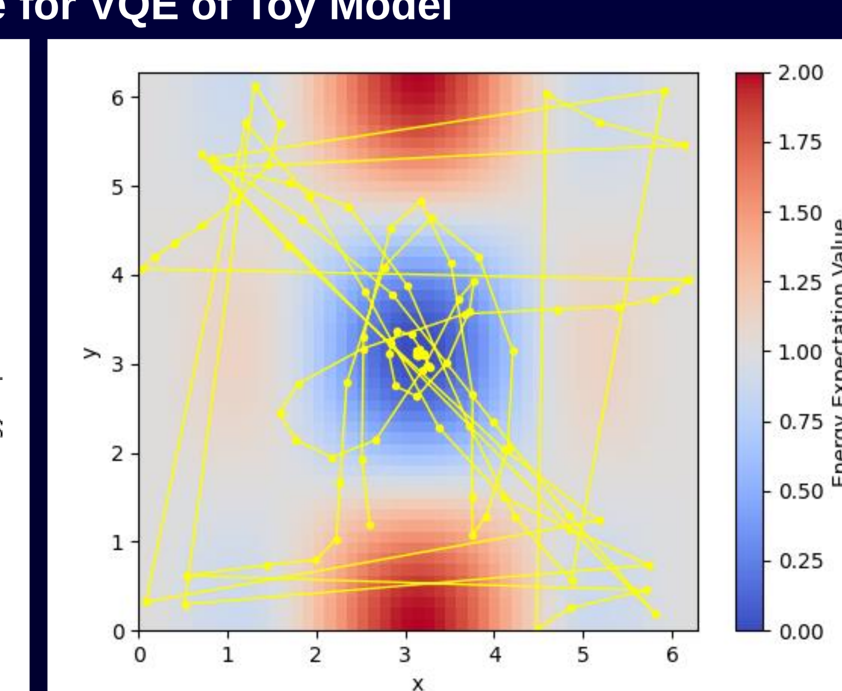



$$H = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Energy Landscape for VQE of Toy Model




Gradient Descent

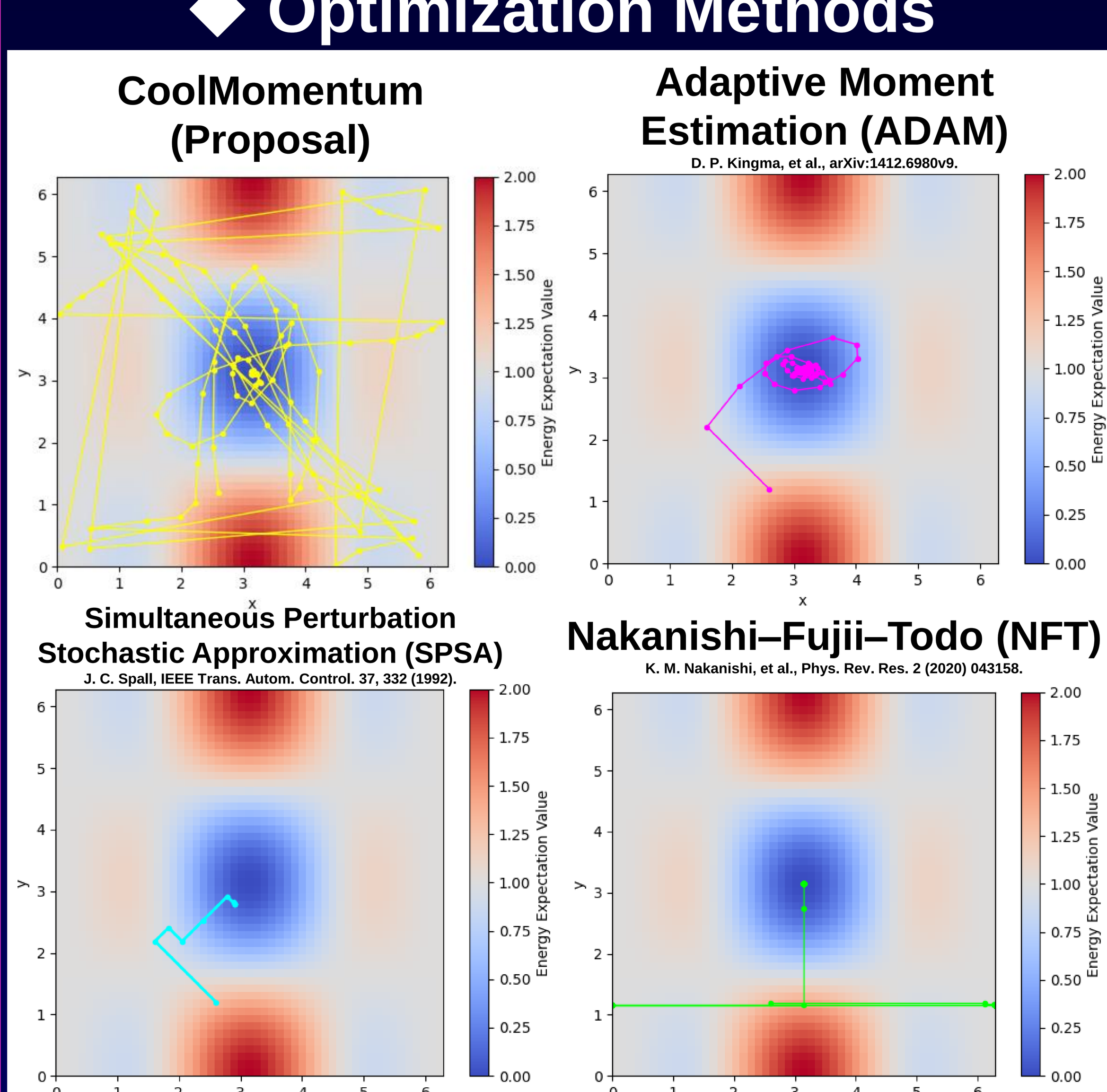



CoolMomentum

✓ Compared to Gradient Descent, CoolMomentum Method Performs Global Search for Solutions before Converging
✓ We Aim to Improve Quality of Converged solutions in VQE by Using Physics-Inspired Methods.
D. Tsukayama, J. Shirakashi and H. Imai, Jpn. J. Appl. Phys. 62 (2023) 088003.

## 3. Experimental Results

### ◆ Optimization Methods




### ◆ Evaluation Metrics in Our Research: Residual Energy $r$

- Sampled Outcome 8192 Times to Estimate $\langle H(\theta)\rangle$
- Initial Values of Parameters were Randomly Sampled from Uniform Distribution $[-\pi, \pi)$.

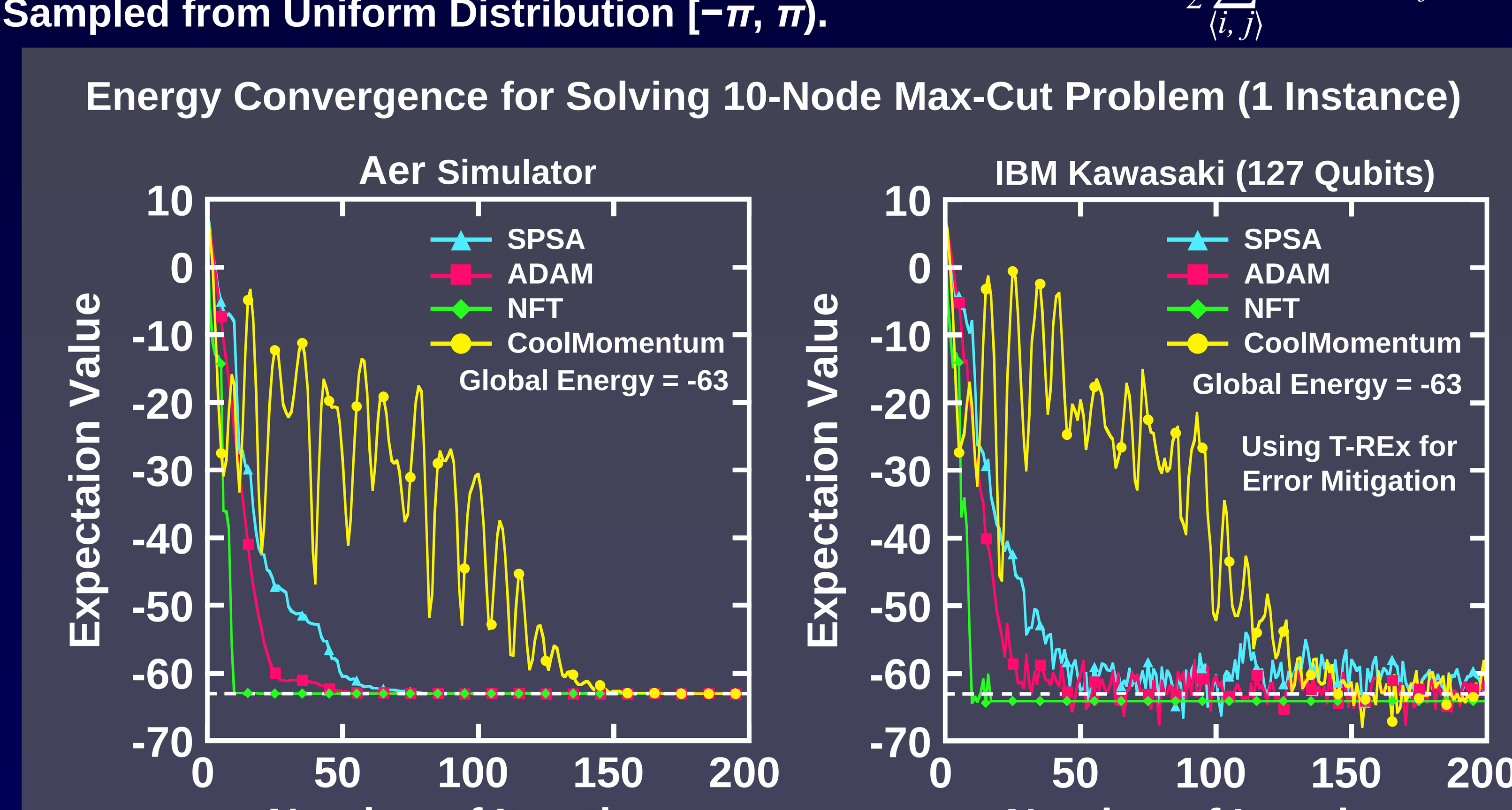
Benchmark: Max-Cut Problem

$$H = -\frac{1}{2}\sum_{\langle i,j\rangle} w_{ij}(I - Z_i Z_j),\ w_{ij} \in [-10, 10]$$

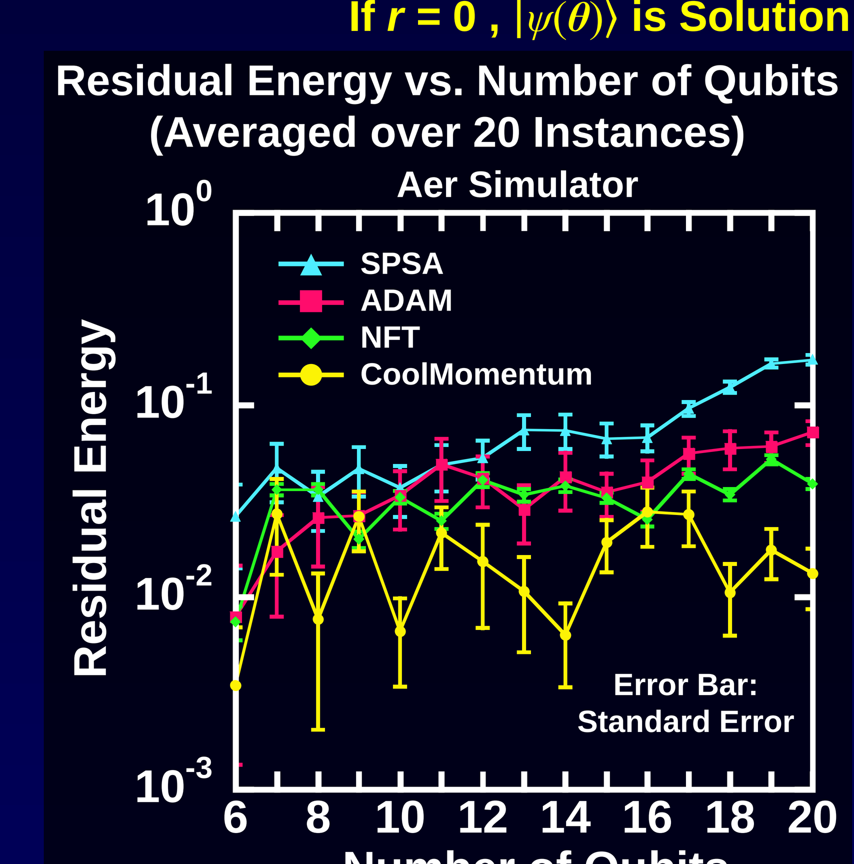
$$r = \frac{\langle H(\theta)\rangle - E_{min}}{E_{max} - E_{min}},\ r \in [0,1]$$

If $r = 0$ , $|\psi(\theta)\rangle$ is Solution

Energy Convergence for Solving 10-Node Max-Cut Problem (1 Instance)




Residual Energy vs. Number of Qubits (Averaged over 20 Instances)




✓ Unlike Other Methods, CoolMomentum Method has Characteristic of Performing Global Search before Energy Converges.
✓ For Most Qubit Numbers, CoolMomentum Method Achieves Lower $r$ and Tends to Find Solutions with Lower Energy.

## 4. Conclusions

- In this study, we solved a Max-Cut problem using VQE with the CoolMomentum optimizer and observed that this strategy achieved higher accuracy than other optimizers, namely ADAM, SPSA, and NFT.
- The convergence characteristics observed when using the error mitigation technique tend to be maintained even when using an actual QPU. This includes our proposed method, the CoolMomentum optimizer.
- While these results provide an initial insight, it is important to note that they are preliminary. The approach we have adopted is novel and uncharted, which necessitates a more comprehensive and rigorous exploration.