

QFw Workflow

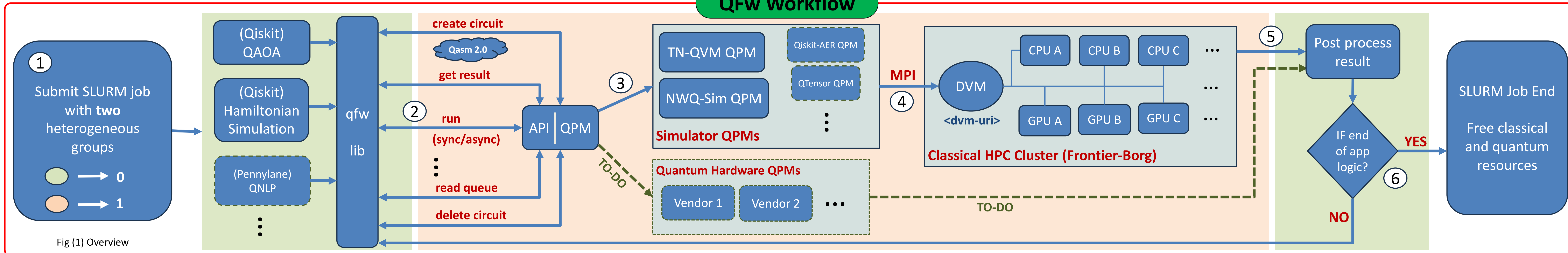


Fig (1) Overview

Motivation

- Quantum Computing (QC) → Efficient for specific problems than classical computing
- Using QC in an HPC environment can be useful for such problems → A Hybrid HPC/QC Computing model
- Resource management** for such a hybrid model is important!

Background

PMIx Reference Runtime Environment (PRRTE) →

- Open-source, **scalable**, and **flexible runtime environment** designed for HPC and parallel computing
- PMIx interfaces with SLURM, PBS and others → **Interoperable**
- Detects and recovers from process and node failures, ensuring continuous and reliable application execution → **Fault-Tolerant**
- Supports rapid job launching, **dynamic** spawning, and process management
- Facilitates efficient execution of parallel applications

PRTE Distributed Virtual Machine (PRTE-DVM) →

- A specific deployment mode of PRRTE that provides a **lightweight DVM** for running parallel applications
- The DVM, identified by a unique **<dvm-uri>**, is responsible for all MPI tasks

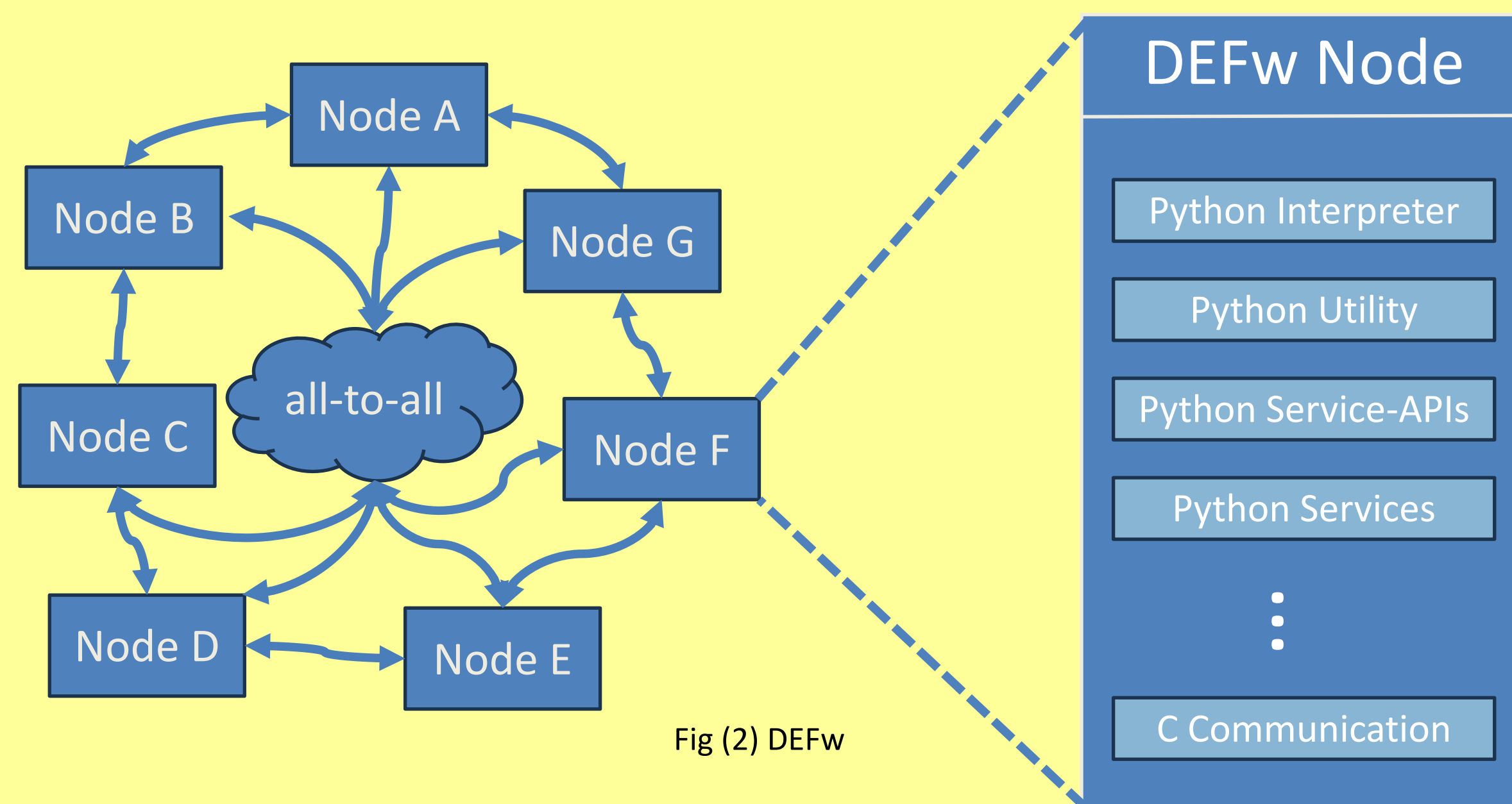


Fig (2) DEFw

Distributed Execution Framework[7] (DEFw) →

- A framework to manage the DVM and the **QFw components**
- DEFw manages all the nodes in the heterogeneous group
- Enables inter-service communication via Remote Procedure Calls (RPCs) **abstracting** it away from each service

QFw Components

Resource Manager

- Keeps track of services running in the DEFw environment
- Respawns services if needed

QPM-API (Quantum Platform Manager)

- Service managing quantum resources
- “Declares” QPM API methods → see Fig (1)
- Supports both synchronous and asynchronous operations

QPM-API-Implementation

- A QPM service (e.g., an HPC Simulator– TN-QVM[1], NWQ-Sim[2]) or actual quantum hardware (our future task using QFw’s plugin architecture)

qfw python library

- Provides functions to connect to QFw and retrieve a resource manager instance, which then gets an QPM API
- QFWSimulator** → Implements Qiskit[3] BackendV2 interface

```
1 # backend_instance = AerSimulator(method="auto")
2 backend_instance = QFWSimulator(simulator="nwqsim")
```

- Pennylane[5]** → Leverages the `pennylane-qiskit` plugin

```
1 import pennylane as qml
2 from qfw.qiskit_integration import QFWSimulator
3 # dev = qml.device('qiskit.aer', wires=2)
4 qfw_backend = QFWSimulator(simulator="nwqsim")
5 dev = qml.device('qiskit.remote', wires=2, backend=qfw_backend)
```

QFw Features

- QFw **decouples** frontends (E.g. Qiskit, Pennylane etc) from backends (E.g. TN-QVM, NWQ-Sim, Qiskit-AER, etc) → see Figure (3) & Figure (6)
- QFw enables application **scaling to multiple nodes** without needing additional code changes → see Fig (3)

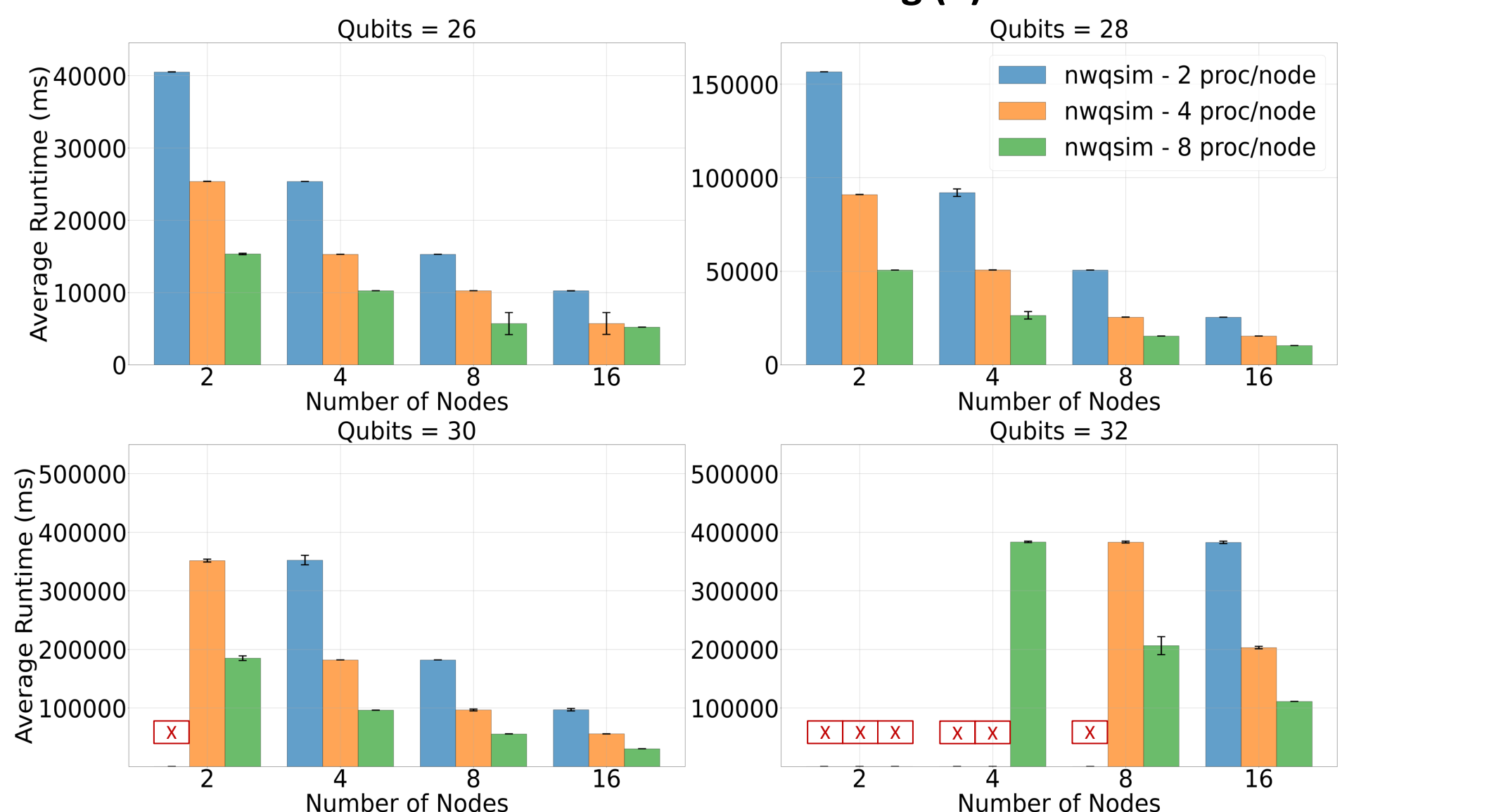


Fig (3) Qiskit GHZ Scale Tests via QFw with NWQ-Sim

- QFw can also run **multiple different circuits in parallel**

- Enables better resource sharing, also useful for certain applications like Distributed-QAOA[6]

- QFw enables **hybrid** application runs
- QFw has some overhead

→ see Fig (4) & Fig (5)
→ see Fig (7)

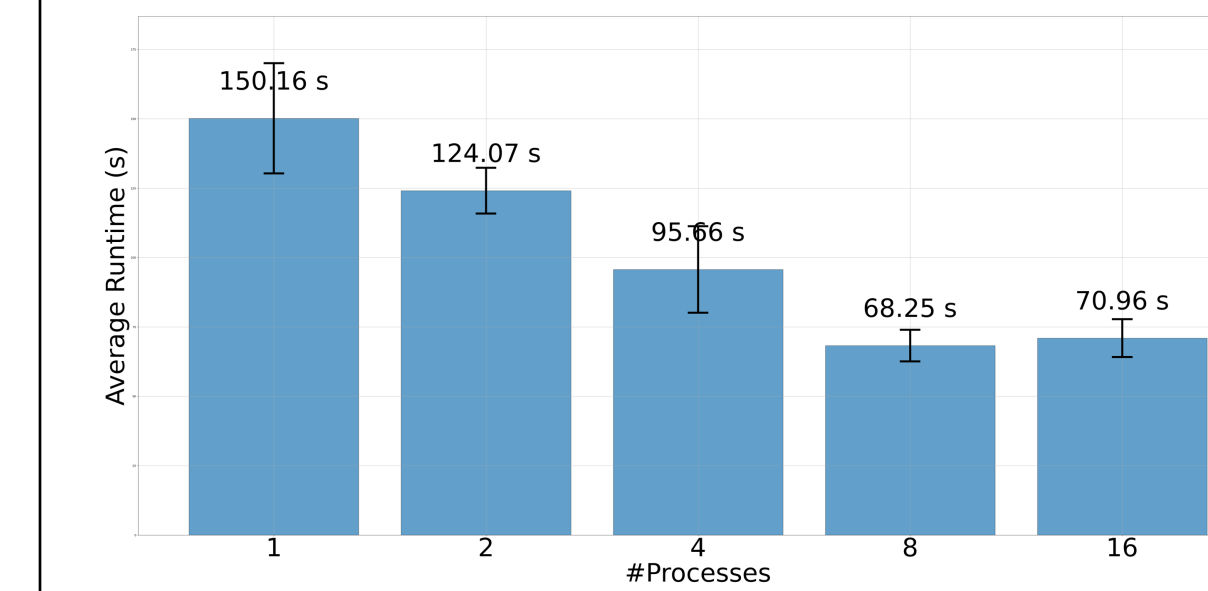


Fig (4) Metamaterial Design[4] QAOA (QUBO 20) via QFw-NWQ-Sim

| QUBO size | Actual Solution | Qiskit-Aer | QFw/NWQ-Sim |
|-----------|-----------------|------------|-------------|
| 4 | -1.070966 | -1.070966 | -1.070967 |
| 8 | -2.367085 | -2.367085 | -2.367085 |
| 10 | -5.102878 | -5.102878 | -5.102878 |
| 16 | -3.974519 | -3.974519 | -3.974519 |
| 20 | -0.934529 | -0.83677 | -0.92976 |

Fig (5) Metamaterial Design[4] QAOA solutions

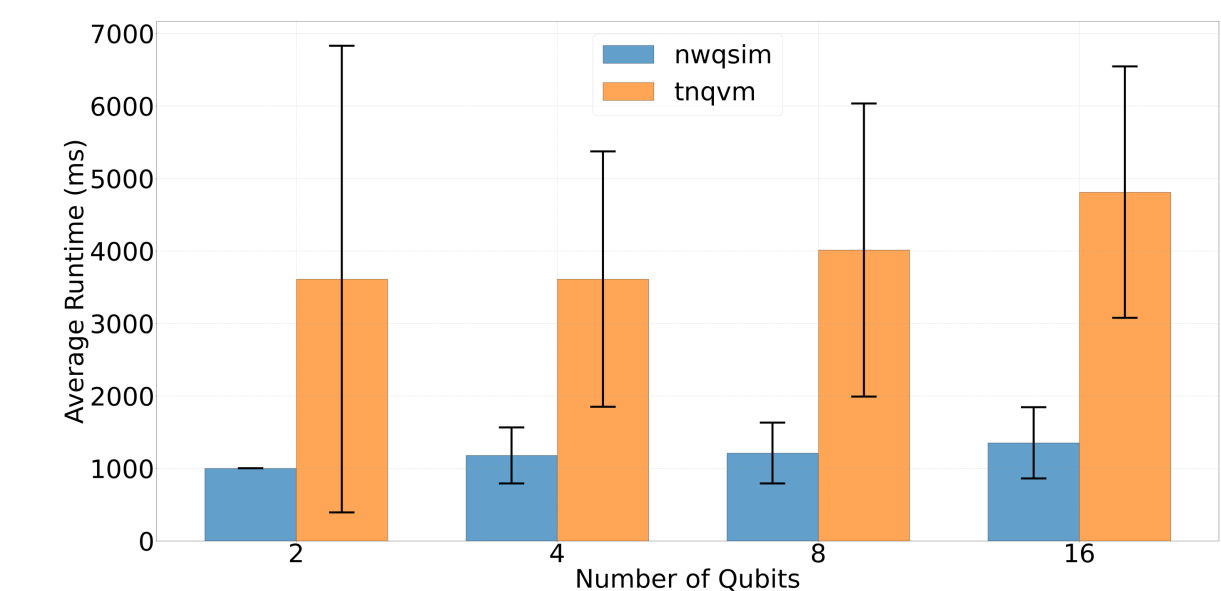


Fig (6) Pennylane GHZ experiments via QFw with NWQ-Sim vs TN-QVM

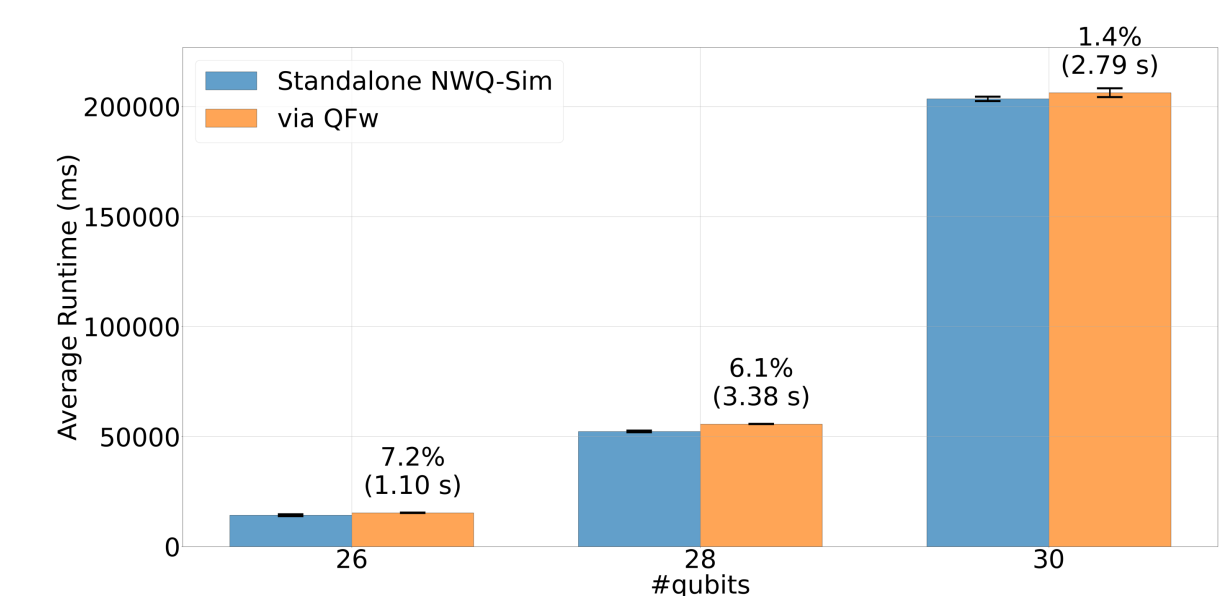


Fig (7) QFw Overhead (GHZ)

Summary & Future

This work 1) integrated **NWQ-Sim** into **QFw**, and 2) introduced a lightweight python layer with the **Qiskit BackendV2 implementation** for **QFw** making it hybrid application friendly. **Next Steps** →

- More QPM-API-Implementations → simulators (qiskit-aer, QTensor), actual quantum hardware!
- Different runs in a hybrid workflow could use different QPMs
- More hybrid applications → E.g., Distributed QAOA[6]
- Auto selection of QPMs based on circuit meta-data
- Smart resource management to avoid wasteful SLURM allocation for QFw (heterogeneous group 1)

References

[1] McCaskey, Alexander J. Tensor Network Quantum Virtual Machine (TNQVM). Computer software. <https://www.osti.gov/servlets/purl/1340180>. Vers. 00. USDOE. 18 Nov. 2016. Web.

[2] Li, A., Fang, B., Granade, C., Prawiroatmodjo, G., Hein, B., Rotteler, M., & Krishnamoorthy, S. (2021). SV-Sim: Scalable PGAS-based State Vector Simulation of Quantum Circuits. Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis.

[3] Javadi-Abhari, A., Treinish, M., Krsulich, K., Wood, C. J., Lishman, J., Gacon, J., Martiel, S., Nation, P. D., Bishop, L. S., Cross, A. W., Johnson, B. R., & Gambetta, J. M. (2024). Quantum computing with Qiskit. <https://doi.org/10.48550/arXiv.2405.08810>

[4] Kim, S., & Suh, I.-S. (2024). Performance Analysis of an Optimization Algorithm for Metamaterial Design on the Integrated High-Performance Computing and Quantum Systems. <https://arxiv.org/abs/2405.02211>

[5] Bergholm, V., Izaac, J., Schuld, M., Gogolin, C., Ahmed, S., Ajith, V., Alam, M. S., Alonso-Linaje, G., AkashNarayanan, B., Asadi, A., Arrazola, J. M., Azad, U., Banning, S., Blank, C., Bromley, T. R., Cordier, B. A., Ceroni, J., Delgado, A., Matteo, O. D., ... Killoran, N. (2022). PennyLane: Automatic differentiation of hybrid quantum-classical computations. <https://arxiv.org/abs/1811.04968>

[6] Kim, S., Luo, T., Lee, E., & Suh, I.-S. (2024). Distributed Quantum Approximate Optimization Algorithm on Integrated High-Performance Computing and Quantum Computing Systems for Large-Scale Optimization. <https://arxiv.org/abs/2407.20212>

[7] Shehata, A., Naughton, T., & Suh, I.-S. (2024). A Framework for Integrating Quantum Simulation and High Performance Computing. <https://arxiv.org/abs/2408.08098>