

# QAOA.jl: Toolkit for the Quantum and Mean-Field Approximate Optimization Algorithms

Tim Bode  ${}^{\circ}$ <sup>1¶</sup>, Dmitry Bagrets<sup>1,2</sup>, Aditi Misra-Spieldenner<sup>3</sup>, Tobias Stollenwerk<sup>1</sup>, and Frank K. Wilhelm<sup>1,3</sup>

1 Institute for Quantum Computing Analytics (PGI-12), Forschungszentrum Jülich, 52425 Jülich, Germany 2 Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany 3 Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany ¶ Corresponding author

#### DOI: 10.21105/joss.05364

#### Software

- Review C<sup>2</sup>
- Repository 🗗
- Archive I<sup>A</sup>

# Editor: Daniel S. Katz 🖒 🗅 Reviewers:

- @babreu-ncsa
- @pkairys
- @Abinashbunty

Submitted: 06 April 2023 Published: 28 June 2023

#### License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License (CC BY 4.0).

### Summary

Quantum algorithms are an area of intensive research thanks to their potential for speeding up certain specific tasks exponentially. However, for the time being, high error rates on the existing hardware realizations preclude the application of many algorithms that are based on the assumption of fault-tolerant quantum computation. On such *noisy intermediate-scale quantum* (NISQ) devices (Preskill, 2018), the exploration of the potential of *heuristic* quantum algorithms has attracted much interest. A leading candidate for solving combinatorial optimization problems is the so-called *Quantum Approximate Optimization Algorithm* (QAOA) (Farhi et al., 2014).

QAOA.jl is a Julia package (Bezanson et al., 2017) that implements the *mean-field Approximate Optimization Algorithm* (mean-field AOA) (Misra-Spieldenner et al., 2023) - a quantum-inspired classical algorithm derived from the QAOA via the mean-field approximation. This novel algorithm is useful in assisting the search for quantum advantage by providing a tool to discriminate (combinatorial) optimization problems that can be solved classically from those that cannot. Note that QAOA.jl has already been used during the research leading to Misra-Spieldenner et al. (2023).

Additionally, QAOA.jl also implements the QAOA efficiently to support the extensive classical simulations typically required in research on the topic. The corresponding parameterized circuits are based on Yao.jl (Luo et al., 2020, 2023) and Zygote.jl (Innes et al., 2019, 2023), making it both fast and automatically differentiable, thus enabling gradient-based optimization. A number of common optimization problems such as MaxCut, the minimum vertex-cover problem, the Sherrington-Kirkpatrick model, and the partition problem are pre-implemented to facilitate scientific benchmarking.

# Statement of need

Demonstration of quantum advantage for a real-world problem is still outstanding. Identifying such a problem and performing the actual demonstration on existing hardware will not be possible without intensive (classical) simulations. QAOA.jl facilitates this exploration by offering a classical baseline through the mean-field AOA, complemented by a fast and versatile implementation of the QAOA. As shown in our benchmarks, QAOA simulations performed with QAOA.jl are significantly faster than those of PennyLane (Bergholm et al., 2018), one of its main competitors in automatically differentiable QAOA implementations. While Tensorflow Quantum (Broughton et al., 2023) supports automatic differentiation, there exists, to the authors's knowledge, no dedicated implementation of the QAOA. The class QAOA offered by



Qiskit (Aleksandrowicz et al., 2019) must be *provided* with a precomputed gradient operator, i.e., it does not feature automatic differentiation out of the box.

# Acknowledgements

The authors acknowledge partial support from the German Federal Ministry of Education and Research, under the funding program "Quantum technologies - from basic research to the market", Contract Numbers 13N15688 (DAQC) and 13N15584 (Q(AI)2) and from the German Federal Ministry of Economics and Climate Protection under contract number 01MQ22001B (Quasim).

## References

- Aleksandrowicz, G., Alexander, T., Barkoutsos, P., Bello, L., Ben-Haim, Y., Bucher, D., Cabrera-Hernández, F. J., Carballo-Franquis, J., Chen, A., Chen, C.-F., & al., et. (2019). *Qiskit: An* open-source framework for quantum computing. https://doi.org/10.5281/zenodo.2562111
- 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., Di Matteo, O., ... Killoran, N. (2018). *PennyLane: Automatic differentiation of hybrid quantum-classical computations*. arXiv. https://doi.org/10.48550/arxiv.1811.04968
- Bezanson, J., Edelman, A., Karpinski, S., & Shah, V. B. (2017). Julia: A fresh approach to numerical computing. SIAM Review, 59(1), 65–98. https://doi.org/10.1137/141000671
- Broughton, M., Verdon, G., McCourt, T., Martinez, A. J., Yoo, J. H., Isakov, S. V., Massey, P., Halavati, R., Niu, M. Y., Zlokapa, A., Peters, E., Lockwood, O., Skolik, A., Jerbi, S., Dunjko, V., Leib, M., Streif, M., Von Dollen, D., Chen, H., ... Mohseni, M. (2023). Tensorflow quantum. In *GitHub repository*. GitHub. https://github.com/tensorflow/quantum
- Farhi, E., Goldstone, J., & Gutmann, S. (2014). A quantum approximate optimization algorithm. ArXiv e-Prints.
- Innes, M., Edelman, A., Fischer, K., Rackauckas, C., Saba, E., Shah, V. B., & Tebbutt, W. (2019). A differentiable programming system to bridge machine learning and scientific computing. arXiv. https://doi.org/10.48550/arxiv.1907.07587
- Innes, M., Edelman, A., Fischer, K., Rackauckas, C., Saba, E., Shah, V. B., & Tebbutt, W. (2023). Zygote.jl. In *GitHub repository*. GitHub. https://github.com/FluxML/Zygote.jl
- Luo, X.-Z., Liu, J.-G., Zhang, P., & Wang, L. (2020). Yao.jl: Extensible, Efficient Framework for Quantum Algorithm Design. *Quantum*, 4, 341. https://doi.org/10.22331/ q-2020-10-11-341
- Luo, X.-Z., Liu, J.-G., Zhang, P., & Wang, L. (2023). Yao.jl. In *GitHub repository*. GitHub. https://github.com/QuantumBFS/Yao.jl
- Misra-Spieldenner, A., Bode, T., Schuhmacher, P. K., Stollenwerk, T., Bagrets, D., & Wilhelm, F. K. (2023). *Mean-field approximate optimization algorithm*. arXiv. https: //doi.org/10.48550/ARXIV.2303.00329
- Preskill, J. (2018). Quantum Computing in the NISQ era and beyond. Quantum, 2, 79. https://doi.org/10.22331/q-2018-08-06-79