Srivathsan Poyyapakkam Sundar

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Summary

Quantum algorithms researcher with a strong background in computational chemistry and materials science. Experienced in developing, implementing, and benchmarking quantum algorithms for ground and excited state modeling, with a focus on scalable and fault-tolerant approaches. Proven track record of cross-functional collaboration, project leadership, and translating complex scientific challenges into quantum algorithmic solutions. Additionally has a keen interest in quantum machine learning.

Experience

Postdoctoral Research Fellow, Quantum Algorithms in Chemistry

University of North Dakota July 2024 – Present

- Led research and development of quantum algorithms for molecular simulations, focusing on ground and excited state problems relevant to chemistry and materials science.
- Designed and implemented quantum subspace expansion and ADAPT-VQE algorithms by developing in-house code using PennyLane and Qiskit.
- Benchmarked and analyzed statistical sampling errors in variational quantum eigensolver (VQE) ansätze, including hardware-efficient, UCCSD, and ADAPT-VQE.
- Collaborated with interdisciplinary teams to port quantum algorithms to IBM Quantum hardware, validating real-world performance and resource requirements.
- Developed and implemented ADAPT-VQE and subspace expansion techniques to accurately model doubly excited states in scalable molecular systems where classical methods are ineffective, demonstrating initial evidence of quantum advantage.
- Presented research at major conferences (APS March Meeting 2025) and published on quantum subspace methods and error analysis.
- Engaged with external partners and contributed to open-source quantum software projects.

Visiting Researcher, Quantum Algorithms in Chemistry

Pacific Northwest National Laboratory (PNNL) June 2025 – Present

- Developing scalable code for the ADAPT-GCIM technique in PennyLane to enable modeling of larger quantum systems such as iron sulfide (FeS) and diuranium U_2.
- Planning implementation and benchmarking of these algorithms on IBM Quantum hardware.
- Contributed to the development of a suite of seven algorithms as part of the research group, including independently developed methods such as UCCSD-VQE, ADAPT-VQE, hardware-efficient ansatz, quantum subspace expansion (QSE), and ADAPT-GCIM.

Self-taught, Quantum Machine Learning

University of North Dakota May 2025 – Present

- Designed and trained hybrid quantum–classical models by integrating parameterized quantum circuits (similar to VQE) with classical neural network layers using PennyLane and TensorFlow.
- Explored feature-mapping strategies for encoding classical data into quantum states to benchmark quantum SVM performance versus classical methods; researched and implemented quantum kernel methods for supervised learning.
- Implemented custom quantum–classical training pipelines by integrating TensorFlow optimizers for quantum circuits, enabling loss-curve visualization and convergence analysis using standard machine learning metrics.
- Documented workflows of code, especially quantum SVM and QNN, in Jupyter notebooks including line-by-line explanations for both beginners and expert users.

Doctor of Philosophy, Computational Chemistry

The University of Melbourne September 2019 – March 2024

- Developed and applied advanced computational models for gas-phase reaction dynamics, including DFT and high-level *ab initio* methods.
- Led projects on vibrational energy calculations, kinetic modeling, and reaction mechanism elucidation for complex chemical systems.
- Integrated quantum chemistry and kinetic modeling tools to address real-world challenges in combustion, interstellar chemistry, and materials growth.

Skills

Quantum Computing: *Qiskit, PennyLane, AWS Braket, Cirq, OpenFermion*
Computational Chemistry: *Gaussian, ORCA, Multiwell*
Kinetic Modelling: *Chemkin, Cantera*
Languages: *Python, MATLAB*

Publications

- **Chemically decisive benchmarks on the path to quantum utility**
  arXiv preprint `https://arxiv.org/pdf/2601.10813`. Submitted to *Chemical Science*
- **On the generalized eigenvalue problem in subspace-based excited state methods for quantum computers**
  arXiv preprint `https://arxiv.org/abs/2503.09670`. Submitted to *J. Chem. Theory Comput.*
- **Effect of statistical sampling errors on Variational Quantum Eigensolver algorithm**
  Conference, APS March Meeting 2025, 2025.
- **Thermal decomposition of Indenyl radical: A theoretical study**
  J. Phys. Chem. A, 2021.
- **PAH Growth in Flames and Space: Formation of Phenalenyl radical**
  J. Phys. Chem. A, 2022.
- **Isotope-specific reactions of acetonitrile with trapped, translationally cold carbon chloride**
  J. Chem. Phys., 2021.
- **Reactions of acetonitrile with trapped, translationally cold acetylene cations**
  J. Phys. Chem. A, 2023.
- **Numerical simulation of spark ignition engine using OPENFOAM**
  Perspectives in Science, 2016.
- **Kinetic modelling of soot formation under ethylene rich laminar premixed flame conditions**
  Conference article, Asia-Pacific Conference on Combustion, Fukuoka, 2019.
- **A study on combustion characteristics of dieseline blend in HCCI Engines**
  Recent Advances in Manufacturing, Automation, Design and Energy Technologies, 2022.

Education

Doctor of Philosophy (PhD), Computational Chemistry

The University of Melbourne, Australia 2024
Awarded Melbourne Research Fellowship to pursue PhD.

Master of Science by Research (MS), Kinetic Modelling

Indian Institute of Technology, Madras, India 2019
Awarded scholarship to pursue Master of Science.

References

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