HPCQS Portfolio of Use-Cases

Added Value of Hybrid Qomputing

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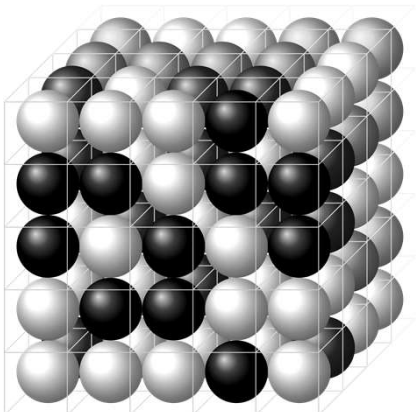
List of HPCQS Use-Cases

1. Simulating Physics Systems
2. Quantum Approximate Optimisation
3. Variational Quantum Eigensolver
4. Quantum Machine Learning

Simulating Physics Systems

1. Lattice-model libraries
   - Generation of arbitrary lattice models
   - Parameterisable geometries and interactions
   - QS/QC platform-agnostic framework for models (1D: chains, 2D: square, triangular, Kagome)
2. Ising model in 1D and 2D
   - Foundational model of statistical and condensed matter physics
   - Study of fundamental physics and material properties
3. Su-Schrieffer-Heege (SSH) model
   - Behaviour of topological insulators (exotic materials with wide-reaching fundamental and applied uses)
4. Strongly correlated materials
   - Avenue to study materials for quantum devices
   - Interest for fundamental physics and applications



A visualization of a 3-D lattice model of a solution consisting of two molecules A and B, here shown as white and black spheres.
Source: Vegar Ottesen, CC BY-SA 3.0)

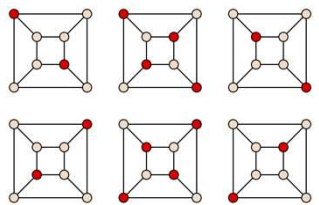
Use-case relevance:

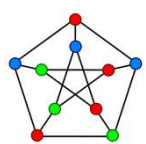
- simulating and understanding quantum effects in many-body systems
- condensed-matter physics
- physical behaviour and material properties, particularly in the fields of energy, electronics and chemistry.

Quantum Approximate Optimisation

1. Combinatorial optimisation library
   - Problem specification, generate quantum schedule and target cost function, perform custom optimisations
   - Target NP-hard combinatorial optimisation problems (e.g. graph colouring, MaxCut, Maximum Independent Set)
2. Unit-Disk Maximum Independent Set
   - Given undirected graph as input
   - Calculate maximum independent set in graph
   - Applications in optimisation problems (e.g. designing stable genetic systems)
3. Factorisation
   - Feasibility and implementability
4. Benchmark QAOA
   - Max-Cut and QUBO problems for benchmarking

Use-case relevance: Combinatorial optimisation problems ubiquitous in science and industry.





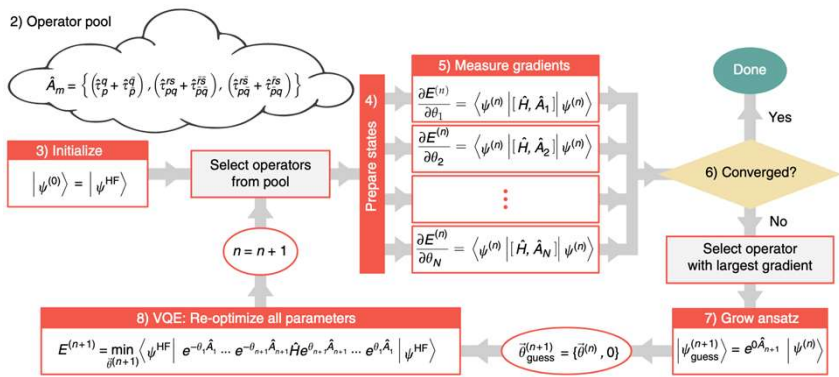
Source: www.ibm.com/thought-leadership/institute-business-value/report/exploring-quantum-financial

Variational Quantum Eigensolver

1. Quantum chemistry benchmarking
   - Electronic structure calculations using techniques like density matrix purification, active-space reduction and truncation of virtual space
2. Catalyst design for nitrogen fixation
   - Study of biological nitrogen fixation by FeMoco, the active site of Mo-dependent nitrogenase
   - Compute kinetics of catalysed reaction, energy intermediates and transition structures
3. Multi-dimensional wave equation problem
   - Solution for partial differential equations
   - VQE-based algorithm for resolution of Helmholtz equation

Use-case relevance:

- Nitrogen fixation problem is relevant to the production of ammonia for fertilisers widely applicable in agriculture
- Wave equations and Helmholtz equation provide deep insight into complex systems such as wave propagation in aerospace industry (noise generation) and O&G/geological sector (study of ground structure)

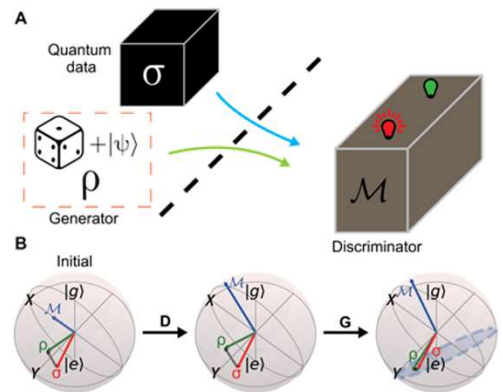


Adaptive VQE

Source: www.nature.com/articles/s41467-019-10988-2.pdf

Quantum Machine Learning

1. Quantum Machine Learning libraries
   - For designing ML algorithms based on quantum generative modelling
   - For supervised learning using quantum states, including encoding, circuits for classifiers
   - For ML algorithms for quantum state estimate and discrimination
2. Reinforcement learning
   - Improved optimisation methods based on reinforcement learning
   - Framework for quantum physics experiments assisted by reinforcement learning
3. Pattern detection
   - Supervised learning approaches on image-based data
4. Classification
   - Supervised learning on data, for instance, from LHC experiments
   - Techniques to control variational hybrid quantum classifier
   - Evaluation on remote sensing image data



Quantum Generative Adversarial Learning
Source: advances.sciencemag.org/content/5/1/eaav2761

Use-case relevance:

- Image recognition, fraud detection, natural language processing, medical diagnosis, FinTech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