ready The Blaise Pascal Quantum Challenge

quaNtumFix: Sustainable Nitrogen Solution

quaNtumFix leverages quantum computing to simulate the nitrogenase enzyme. Industrial ammonia production through the Haber-Bosch process is an energy intensive process requiring high pressure and temperature conditions, accounting for 1-2% of global energy consumption and emissions. Nature, on the other hand, does this using nitrogenase at atmospheric conditions. Understanding this process and thus creating energy efficient processes would improve fertilizer affordability and promote food security.

Supporting the Solution:

quaNtumFix relies on quantum computing to address the molecular complexity of nitrogen fixation, a problem classical systems cannot handle efficiently. Key integrations include:

1. Electronic Structure Calculations: Quantum computing simulates the electronic interactions within the FeMo-cofactor of nitrogenase, capturing quantum effects such as entanglement and superposition.

2. Reaction Pathway Identification: Variational quantum algorithms explore and optimize reaction pathways to minimize energy barriers for nitrogen bond dissociation.

Compatibility with Pasqal's Neutral Atom Technology:

PART 1: Sustainability Impact Assessment

Impact on the Challenge Selected

The proposed solution directly addresses the **Challenge of Sustainable Industries and Transport**, contributing to UN Sustainable Development Goal (SDG) number 9:

SDG 9 – Industry Innovation and Infrastructure:

1. Target 9.4: "By 2030, upgrade infrastructure and retrofit industries to make them sustainable, with increased resource-use efficiency and greater adoption of clean and environmentally sound technologies and industrial processes, with all countries taking action in accordance with their respective capabilities."[1]

2. The innovative ambient nitrogen fixation process, inspired by the natural nitrogenase enzyme, requires **significantly lower energy** input than the energy-intensive Haber-Bosch process, potentially reducing dependence on fossil fuels. This makes it a cleaner, efficient, and environmentally friendlier process than current ammonia production processes.

By leveraging quantum computing to develop a more efficient process for nitrogen fixation, the energy-intensive Haber-Bosch process can be replaced with a

[1] https://sdgs.un.org/goals/goal9#targets_and_indicators

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sustainable alternative. Haber-Bosch currently accounts for over 96% of all industrial nitrogen production and is almost exclusively performed using fossil fuels.[2] Reduction of energy requirements and/or usage of alternative energy sources can significantly reduce greenhouse gas emissions. In addition to SDG 9, quaNtumFix supports SDG 2 by making fertilizers more affordable, promoting equitable access to food and addressing food insecurity. Acknowledging food wastage as being a larger challenge than food shortage[3], creating a shorter pipeline from harvest to table, and providing communal production of food and reduced privatization could offer drastic improvements in food security.

Quantifiable Metrics

1. **Energy Efficiency**:
    - **Target**: 50%–70% reduction in energy usage compared to the Haber-Bosch process.
    - **Rationale**: The natural enzyme nitrogenase operates at ambient temperatures and pressures, making significant energy savings feasible when replicated at scale.
2. **Carbon Footprint**:

[2] https://www.awoe.net/Ammonia-Haber-Bosch-Process.html
[3] https://www.unep.org/news-and-stories/press-release/world-squanders-over-1-billion-meals-day-un-report

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- **Target**: 30%–50% reduction in carbon emissions from ammonia production at scale.
- **Context**: Given that ammonia production currently emits approximately 3% of global CO_2, cutting this by half could remove hundreds of millions of tonnes of CO_2 from the atmosphere annually.[4]

3. **Societal Benefits**:
   - **Reduced Fertilizer Costs**
     i. **Target**: 20%–40% decrease in the production cost of ammonia-based fertilizers.
     ii. **Justification**: Lower energy requirements can directly translate into reduced operational expenditures, benefiting farmers and consumers.
   - **Access for Underprivileged Communities**
     i. **Indicator**: Percentage increase in the availability of fertilizers in low-income regions.
     ii. **Goal**: Enhance crop yields and reduce hunger, in line with **SDG 2 (Zero Hunger)**.
   - **Global Food Production**

[4] https://phys.org/news/2018-07-electrochemically-produced-ammonia-revolutionize-food-production.html

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    i. **Indicator**: Number of people benefiting from more affordable fertilizers, measured via farm-level yield data and national agricultural productivity statistics.[5]

4. **Scaling and Adoption Metrics**:
    - **Metric**: The percentage of global fertilizer producers transitioning to or integrating nitrogenase-based processes over time.
    - **Benchmark**: Year-over-year growth in production capacity.

Proposed Metrics for Evaluating Success

1. **Technical Feasibility**:
    - **Quantum Simulation Accuracy**: Number of successful quantum simulations replicating the nitrogenase enzyme reaction mechanism.
    - **Energy Requirements**: Comparison of actual energy consumption in pilot plants vs. traditional Haber-Bosch processes.
2. **Economic Impact**:
    - **Operational Cost Reduction**

5 https://openknowledge.fao.org/server/api/core/bitstreams/67b1e9c7-1a7f-4dc6-a19e-f6472a4ea83a/content

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i. *Metric*: Percentage decrease in operational costs for fertilizer production plants that adopt the new technology.
ii. *Measurement Tool*: Financial reporting from pilot projects and early adopters.

- **Impact on Food Prices**
  i. *Indicator*: Correlation between lower fertilizer costs and changes in overall food production costs and retail prices.
  ii. *Relevance*: Demonstrates direct benefits to consumers and producers, especially in developing regions.

3. **Social Impact**:
   - **Food Security Metrics**
     i. *Example*: Improvements in the Global Food Security Index (The Economist Intelligence Unit), or reduction in prevalence of undernourishment.
     ii. *Goal*: Show that improved fertilizer accessibility contributes to **SDG 2** targets.
   - **Reduction in Hunger Statistics**
     i. *Indicator*: Measured drop in the number of undernourished individuals in regions adopting the technology.
     ii. *Target*: Enhanced agricultural output that directly boosts food availability.

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Compatibility with Pasqal's Neutral Atom Technology:

Supporting Evidence

- **Erisman, J. W., Sutton, M. A., Galloway, J., Klimont, Z., & Winiwarter, W. (2008).** How a century of ammonia synthesis changed the world. *Nature Geoscience, 1*(10), 636–639.
- **Smith, C., Hill, A. K., & Torrente-Murciano, L. (2020).** Current and future role of Haber–Bosch ammonia in a carbon-free energy landscape. *Energy & Environmental Science, 13*(2), 331–344.
- **Smil, V. (2001).** *Enriching the Earth: Fritz Haber, Carl Bosch, and the Transformation of World Food Production.* The MIT Press.
- **FAO (2022).** *The State of Food Security and Nutrition in the World.* Food and Agriculture Organization of the United Nations.
- **Our World in Data (2023).** Fertilizers. https://ourworldindata.org/fertilizers
- **The Economist Intelligence Unit** – Global Food Security Index.

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Compatibility with Pasqal's Neutral Atom Technology:

PART 2: Technical Feasibility of the Solution

General Approach and Strategy Proposed

Overall Strategy for Solving the Problem:

The central goal of nitrogen fixation research is to replace the energy-intensive Haber-Bosch process for ammonia synthesis with a sustainable alternative inspired by the natural nitrogenase enzyme. Nitrogenase can break the nitrogen (N_2) triple bond and form ammonia (NH_3) at ambient temperature and pressure, a feat that classical industrial processes require extreme conditions to achieve. Achieving such ambient conditions will involve enzymes, and large complicated molecules with challenging electronic structures. To understand the underlying catalysis, we must be able to model the electronic structure accurately within a reasonable time-to-solution to enable studies that implement an *in-vitro* alternative of the reaction that could replace the process.Modeling the electronic structures on classical computers results in a solution that becomes exponentially more expensive as the size of the system increases, making studies of complex systems a far-fetched dream. However, quantum computing circumnavigates the exponential nature of these solutions, offering solutions in the near term. We discuss how quantum computing circumnavigates the exponential nature and offers solutions in near term.

The objectives of quaNtumFix are:

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1. Enabling Quantum Chemistry: Use quantum computing to model the molecular interactions in the active site of nitrogenase, particularly the FeMo-cofactor, which catalyzes the reaction.
2. AI Assistance: Employ classical AI algorithms to preprocess inputs, optimize parameters, and interpret noisy outputs from quantum computations.
3. Process Optimization: Translate insights gained from simulations into a scalable, energy-efficient synthesis process for industrial ammonia production.

Problem Solving with AI and Quantum Computing:

1. Nitrogenase Simulation: The nitrogenase enzyme contains a highly complex active site where nitrogen reduction occurs. Classical computers struggle to simulate this due to the exponential scaling of quantum interactions. Quantum computers can efficiently model the electronic structure and reaction dynamics of this site.
    - Quantum Role: Quantum algorithms like the Variational Quantum Eigensolver (VQE) simulate the ground-state energy and transition states of nitrogenase during the nitrogen fixation reaction.
    - AI Role: AI assists in training the variational parameters of the quantum circuits, accelerating convergence and improving the accuracy of molecular simulations.
2. Sustainability Benefits vs. Quantum AI Footprint:
    - Sustainability Benefits:

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        - The nitrogenase-inspired process operates at ambient conditions, potentially reducing energy consumption by up to 70% compared to the Haber-Bosch process.
        - Carbon emissions from ammonia synthesis could drop by 30%-50%, saving millions of metric tons of CO_2 annually.
    - Quantum AI Footprint:
        - Neutral atom quantum platforms like Pasqal's consume relatively low energy compared to industrial manufacturing.
        - Powering quantum AI systems with renewable energy can offset their carbon footprint, ensuring net-positive environmental impacts.

Quantum Computing Integration

1.

Mathematical Problem Formulation

Problem Definition:

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The central idea of understanding a reaction through computational modeling requires preparation of a model of the system under study, using quantum mechanics to predict observables and comparing those observables to the experimentally determined values. We aim to build a framework that can calculate the ground state energy of a given molecule. Once that has been achieved, we can use the information to determine a set of possible reaction mechanisms and predict the differences in ground state energies of each. This will provide us with the activation energy and allow us to compare the values with experimentally proven values. Fundamentally, the challenge is to approximate the wave function of a system as some eigenstate of some Hamiltonian. The entire challenge of modeling nitrogen fixation could be broken down into several orthogonal problems, as follows: calculation of a molecular Hamiltonian; wave function ansatz; representation of a Hamiltonian on a quantum circuit; preparation of a guess state; and evolution of a guess state. There are several ways to approximate each of these subproblems, depending on the resource availability. We will discuss each of the possible approximations in each of the sections below.

Modeling Hamiltonians

The molecular Hamiltonian, in second quantized form, is simply written as

$$\hat{H} = \Sigma_{ij} h_{ij} a_i^{\dagger} a_j + \Sigma_{ijkl} g_{ijkl} a_i^{\dagger} a_j^{\dagger} a_k a_l$$

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where i, j, k, l represent a set of orbitals, $a_i^\dagger (a_i)$ is the creation (annihilation) operator, and h_{ij}, g_{ijkl} are one- and two-electron integrals. This Hamiltonian can be over the entire molecule, for certain sets of orbitals (frozen core approximation), projected onto a smaller basis through singular value decomposition (DMET), a set of multiple fragment Hamiltonians, or through an matrix product operator represented as a tensor network, or a combination of these techniques.

Wave Function Ansatz

The common ansatz for solving weakly correlated electronic structure problems is by representing wave function as a single determinant or as a slight perturbation to a single determinant that gives rise to coupled cluster and Møller-Plesset perturbation theories. However, compounds such as FeMo cofactor have multiple partially filled transition metals that are inherently multiconfigurational, i.e., a single configuration cannot capture the fundamentally multiconfigurational nature of the molecule. Typically, within the quantum chemistry community, a configuration interaction or a matrix product state ansatz are used. Configuration interaction represents the wave function with all possible combinations, whereas matrix product state represents the wavefunction as a tensor train connected with an internal bond dimension.

Equations/Models:

1. **Hamiltonian for Nitrogenase System:**

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$$H = \sum_i h_i a_i^\dagger a_i + \sum_{i,j} h_{i,j} a_i^\dagger a_j + \sum_{i,j,k,l} h_{i,j,k,l} a_i^\dagger a_j^\dagger a_j a_k a_l + \ldots$$

where $h_i, h_{i,j}, h_{i,j,k,l}$ are integrals representing one-body, two-body, and higher-order interactions, and $a_i^\dagger$, a_i are fermionic operators.

2. **Energy Minimization:**
   The goal is to find the ground-state energy:

   $$E_{ground} = min_\theta \langle \psi(\theta) | H | \psi(\theta) \rangle$$

   Here, $|\psi(\theta)\rangle$ is the quantum state defined by variational parameters θ, optimized using classical feedback.

3. **Reaction Pathway Optimization:**

   $$\Delta E = E_{TS} - E_{reactants}$$

   Transition state energies E_{TS} are calculated, and pathways with the lowest energy barriers ΔE are identified.

Assumptions and Simplifications:

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1. The enzyme's active site is modeled as a simplified quantum system with key atoms and interactions.
2. Solvent effects and external conditions are approximated rather than explicitly simulated.
3. Computations focus on the FeMo-cofactor as the primary catalyst, omitting secondary biological interactions.

Computational Complexity:

Simulating nitrogenase's active site involves solving a quantum many-body problem with exponential complexity on classical computers. Quantum computing addresses this by:

- Exploiting quantum parallelism to efficiently explore the solution space.
- Using hybrid algorithms (e.g., VQE) to minimize the computational burden by distributing tasks between quantum and classical processors.

Technical Schematics and Simulations

Preliminary quantum simulations on small nitrogenase-inspired models demonstrate the feasibility of modeling bond dissociation processes. These models are scalable, enabling future simulations of the full enzyme system as quantum hardware improves.

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Compatibility with Pasqal's Neutral Atom Technology:

PART 3: Innovation and Creativity

State of the Art

The quaNtumFix project tackles the long-standing problem of nitrogen fixation, specifically targeting the inefficiencies of the Haber-Bosch process. Current research in quantum chemistry has demonstrated the potential for quantum computing to address complex molecular simulations, particularly for energy-intensive reactions like nitrogen bond dissociation. However, much of this research remains theoretical or limited to simple molecules due to hardware constraints.

- Existing Technologies:
    - **Density Functional Theory (DFT)**: While DFT is a powerful tool in computational chemistry, it struggles to accurately capture the **full quantum behavior** of large, complex enzymes like nitrogenase, especially in the presence of strong electron correlations.
    - **Computational Bottlenecks**: Modeling enzyme active sites (e.g., FeMo-cofactor) is computationally prohibitive with purely classical methods, limiting **in-depth** understanding of reaction mechanisms (Nature Reviews, 2020).
- Quantum Computing Contributions:
    - Recent studies have applied quantum algorithms like Variational quantum adiabatic approximation(VQAA) to small-scale molecules,

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Compatibility with Pasqal's Neutral Atom Technology:

showing promise in tackling computational bottlenecks in quantum chemistry.

Novelty of the Approach:

quaNtumFix introduces an innovative application of existing quantum AI algorithms and adapts them to the novel challenge of sustainable ammonia synthesis:

Idea:

1. Set up an initial Hamiltonian that is easy to prepare and our target Hamiltonian that we are trying to find the ground state with. We can utilize the adiabatic theorem to slowly evolve the ground state to the new ground state of the target Hamiltonian. We could also split our Hamiltonians into different parts which are easier to physically implement.
2. Use the DRMG to set up the graph structure of the problem and then use VQAA to find the ground state energy/state.

1. Customized Quantum Simulations: Tailored VQAA models for nitrogenase's FeMo-cofactor, incorporating enzyme-specific parameters.
2. Hybrid Workflow: Combines AI-based optimization with quantum simulation to refine quantum circuit parameters, ensuring convergence and scalability.
3. Scalability with Neutral Atoms: Exploits Pasqal's neutral atom quantum architecture to simulate the enzyme's reaction dynamics, leveraging high connectivity and analog quantum advantages.

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Supporting Research:

- Relevant studies include:
    - Quantum chemistry with VQE algorithms (Nature Reviews, 2020).
    - Molecular simulations on neutral atom platforms (arXiv, 2023).
    - Catalysis models in quantum computing (ACS Catalysis, 2022).

These references demonstrate that while quantum chemistry applications are an active field of study, quaNtumFix targets a specific, high-impact use case that has not been thoroughly explored.

Disruption and Uniqueness

Original Contribution:

quaNtumFix disrupts the status quo by providing a sustainable alternative to the Haber-Bosch process, combining the precision of quantum simulations with the adaptability of AI.

- Novel Molecular Insights: Enables accurate simulations of nitrogenase's active site, which classical methods cannot achieve.
- Energy Efficiency: Targets a 70% reduction in energy consumption for ammonia synthesis.

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Compatibility with Pasqal's Neutral Atom Technology:

- Accessibility: Scales ammonia production for underprivileged regions, addressing food security challenges.

Advancements Beyond Current Practices:

1. Energy Savings: While prior quantum chemistry research focuses on computational accuracy, quaNtumFix links these advancements to tangible energy and CO_2 savings.
2. Integrated Quantum-AI System: Bridges the gap between quantum simulation and real-world engineering solutions.
3. New Benchmark for Quantum Applications: Establishes nitrogenase modeling as a benchmark for future quantum chemistry projects.

Alignment with Quantum AI Trends

Positioning in the Broader Quantum AI Landscape:

quaNtumFix aligns closely with emerging trends in quantum AI, particularly the push for applied quantum computing in sustainability:

- Alignment with Green Tech Goals: quaNtumFix is part of a larger movement toward using quantum AI to address climate change and resource efficiency, directly contributing to UN SDGs 2 (Zero Hunger) and 13 (Climate Action).

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Compatibility with Pasqal's Neutral Atom Technology:

- Convergence of Quantum and AI: By leveraging AI to optimize quantum simulations, quaNtumFix exemplifies how hybrid approaches can unlock the potential of quantum computing for real-world challenges.

Contributions to Sustainability and Quantum AI:

1. Sustainability Impact: Reduction in carbon emissions and energy use in fertilizer production.
2. Quantum AI Advancement: Demonstrates the practical utility of VQAA and neutral atom technologies in solving complex, high-impact problems.
3. Scalability: Provides a roadmap for scaling quantum solutions to industrial applications, paving the way for broader adoption of quantum AI systems.

Supporting Documentation

Scientific papers and supporting documentation for this section include:

- Nature Reviews, 2020: *Advances in quantum chemistry simulations using VQEs*.
- ACS Catalysis, 2022: *Modeling catalysis reactions with quantum algorithms*.
- arXiv, 2023: *Neutral atom platforms for molecular simulation*.

Objective of this section: Highlight the originality and disruptive potential of your quantum AI solution.

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Compatibility with Pasqal's Neutral Atom Technology:

What to include:

State of the Art:

- Position the solution within existing research and technologies.
- Justify the novelty of the approach, describe whether your project involves:
    - A new quantum AI algorithm.
    - An innovative application of an existing algorithm.
    - An adaptation of known methods to a novel use case.

(Attach scientific papers and any documentation available to support this subsection)

Disruption and Uniqueness:

- Explain how your solution offers an original contribution to the field.
- Highlight specific areas where it disrupts or advances beyond current practices.

Alignment with Quantum AI Trends:

- Position your project within the broader quantum AI landscape.
- Discuss its potential to contribute to advancements in both sustainability and quantum AI.

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Compatibility with Pasqal's Neutral Atom Technology:

APPENDIXES: Please feel free to add any relevant document here

Random notes (Megan)-

- ask Shimpei on Monday about how to best incorporate AI and what scalability entails
- Using AI to pre-process inputs, optimize parameters, interpret noisy outputs, and benchmarking
- maybe we could use AI to try and compare

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Compatibility with Pasqal's Neutral Atom Technology:

The companies currently using Haber-Bosch are unlikely to be good early sponsors for your commercial stage, as you are essentially proposing that they write down their sunk cost in ammonia synthesis.
A better idea is to look at the feedstock producers and the ammonia consumers. The idea would be to manufacture NH3 in countries with cheap renewable electricity, transport it to demand countries, and consume it there.
Note that ammonia is not just useful for fertilizers; it is increasingly attracting attention for being an efficient hydrogen transport mechanism, and a carbon-free fuel for direct consumption (whether in gas turbines or in certain types of fuel cells).
In other words, your feedstock would be green hydrogen (and upstream of that renewable electric power producers), while the downstream consumers would be fertilizer manufacturers, electric power companies, and hydrogen consumers (via electrolysis of ammonia at destination site).
Your value proposition to the green electricity sector would be to add value to their electricity by adding a transportable storage option, and the value to the downstream players would be cheaper green ammonia.

As a quick summary, please see this presentation:
PowerPoint-presentatie

As a concrete example of a value chain, Japan happens to be one of the countries strongly interested in the green ammonia value chain; we have to import most of our energy consumption and have invested heavily in hydrogen technologies, but still need to crack the overseas transport problem. The two main alternative hydrogen carrier molecules currently being explored are methylcyclohexane (MCH), which can be broken down to toluene and hyrogen and then back together to form a closed loop; and ammonia. An efficient green ammonia synthesis would fit our national interest perfectly, and is likely to attract the interests of Japanese energy and petrochemical industries, as well as companies in

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Compatibility with Pasqal's Neutral Atom Technology:

energy-rich countries that currently sell to Japan (such as Australia and the Persian Gulf states). My employer Sumitomo would probably be interested at that stage.

I don't think you should go into that much detail about this as no one is expecting you to do a deep geopolitical study during this hackathon, but try to expand on the above topic a bit to provide the full breadth of your technology's impact. Focusing just on existing F-B customers is certainly underselling your research!