Mathematical Challenges in Adaptation of Quantum Chemistry to Quantum Computers - 23w2015

Sergey Gusarov (National Research Council Canada),
James Brown (Good Chemistry Company),
Prashant Nair (UBC),
Valera Veryazov (Lund University)

September 1–3, 2023

1 Introduction

The "Mathematical Challenges in Adaptation of Quantum Chemistry to Quantum Computers" workshop, held in Banff, Alberta, from September 1 to September 3, 2023, was a significant event that brought together experts from various fields to discuss the intersection of quantum chemistry, mathematics, and quantum computing. The workshop aimed to address the current mathematical and computational challenges in quantum chemistry and explore how modern hardware architectures, particularly quantum computers, can revolutionize this field. The presentations jointly covered a wide range of topics, from quantum computing fundamentals to practical applications in quantum chemistry and related fields, offering attendees a comprehensive view of the mathematical and computational challenges and opportunities at the intersection of quantum chemistry and quantum computing.

2 Recent Developments and Open Problems

The workshop was more than just a series of presentations and discussions; it was an affirmation of the exponential advancements and possibilities that lie at the intersection of quantum computing and quantum chemistry. The event stood out as a testament to the dedication and passion of the global scientific community, striving to bridge gaps and foster collaborations in these rapidly evolving fields. In a world where technology is advancing at an unprecedented pace, such gatherings become crucial platforms for cross-disciplinary dialogue, bridging theoretical frameworks with practical applications. They represent not just the exchange of knowledge but the synthesis of new ideas that have the potential to drive forward both scientific understanding and technological innovation. Quantum computing, with its potential to process and analyze vast amounts of data in ways previously thought impossible, promises to be the key that unlocks many of quantum chemistry's most intricate puzzles. From simulating complex molecular interactions to accelerating the discovery of new materials and pharmaceuticals, the potential applications of this synergy are vast and varied. However, with these advancements come challenges that require not just technical prowess but also visionary thinking and robust collaboration. The workshop highlighted the necessity of an interdisciplinary approach, where experts from diverse backgrounds—be it physics, chemistry, mathematics, or computer science—come together to share insights and craft solutions that no single discipline could achieve on its own.

Moreover, the workshop echoed a broader sentiment prevalent in the scientific community: the importance of constant learning and adaptability. As the lines between disciplines blur and new challenges emerge, the need to stay updated, reevaluate traditional methodologies, and be open to novel approaches becomes more critical than ever.

3 Key Takeaways:

1. Quantum Advantage: The workshop reiterated the concept of a "quantum advantage" in quantum chemistry. Quantum computers have the potential to perform calculations exponentially faster than classical computers in specific areas of quantum chemistry, offering the promise of groundbreaking advancements in simulating molecular structures and chemical reactions. Multiple presentations highlighted recent accomplishments, encompassing novel methodologies, advancements in software development, and the utilization of quantum machine learning for tackling the Schrödinger equation.
2. Optimization Challenges: Quantum chemistry often involves complex optimization problems. While quantum computers hold the promise of solving these problems efficiently, there is a continued need for the development of efficient quantum optimization algorithms. The discussions revolved around the significance of quantum optimization and explored emerging directions in its application to quantum chemistry.
3. Interdisciplinary Collaboration: A recurring theme throughout the workshop was the critical importance of interdisciplinary collaboration. Success in adapting quantum chemistry to quantum computers hinges on cooperation between quantum physicists, chemists, mathematicians, and computer scientists. These multidisciplinary teams are at the forefront of developing and testing quantum algorithms and applications.
4. Real-World Applications: The integration of quantum chemistry with quantum computers has far-reaching implications across various industries, including pharmaceuticals, materials science, and environmental science. Quantum computing can accelerate drug discovery, aid in designing new materials, and enhance our understanding of complex chemical processes.

4 Scientific Progress Made

The "Mathematical Challenges in Adaptation of Quantum Chemistry to Quantum Computers" workshop was a resounding success, emphasizing the transformative potential of quantum computing in the field of quantum chemistry. It provided a forum for in-depth discussions, knowledge sharing, and the exploration of cutting-edge research in this exciting interdisciplinary domain. This workshop underscored the critical role that collaboration and innovation play in advancing the boundaries of science and technology. The organizers, presenters, and participants contributed significantly to making this event a valuable platform for the exchange of ideas and the pursuit of groundbreaking solutions. As we look to the future, it is evident that the integration of quantum chemistry and quantum computing will continue to push the boundaries of scientific discovery, leading to new frontiers in understanding the quantum world and addressing complex computational challenges.

5 Outcome of the Meeting

In conclusion, the "Mathematical Challenges in Adaptation of Quantum Chemistry to Quantum Computers" workshop was not just an event, but a milestone in the ongoing journey of scientific exploration and discovery. As attendees returned to their respective institutions, they carried with them not just the knowledge acquired but also a renewed sense of purpose and commitment to the collective goal of pushing the boundaries of what's possible in quantum chemistry and quantum computing. The ripple effects of this gathering will undoubtedly be felt in research papers, collaborations, and breakthroughs in the years to come, further solidifying the workshop's importance and impact on the global scientific landscape. The workshop holds great significance for Canadian research, as it serves as a focal point for advancing the country's contributions to the field of quantum chemistry and quantum computing. Also, it serves as a catalyst for enhancing both the quality and reach of Canadian research by promoting fruitful collaborations between Canadian scientists

and leading experts from around the world. This collaborative spirit is fundamental in driving advancements in quantum chemistry and quantum computing on a global scale.