Centre for Research in Molecular Modeling
CERMM
Centre de recherche en modélisation moléculaire

UNIVERSITÉ Concordia UNIVERSITY

Lecture within the International Graduate Summer School – Modeling and Simulations Across the Molecular Sciences and Engineering

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Technologies on the Rise: Quantum Computing

Quantum computers have the potential to be more powerful than classical computers. For example, simulating quantum mechanics on a classical computer is extremely unnatural: solving the Schrödinger equation exactly for 100 spin-1/2 particles on a classical computer involves a Hamiltonian matrix of size $(2^{100}) \times (2^{100})$, which has 10^{60} elements. Quantum computers can intrinsically take care of quantum mechanics at the hardware level, rather than trying to simulate it with classical hardware. Quantum hardware now exists with 2048 qubits. This hardware is designed to find the ground state of a 2048-spin Hamiltonian with programmable couplings between the spins -- a task that classically would require finding the lowest eigenvalue of a $(2^{2048}) \times (2^{2048})$ matrix containing over 10^{1000} elements. If we can avoid storing $(2^N) \times (2^N)$ matrices by instead having only N qubits, we should also be able to solve very large linear algebra problems having nothing to do with quantum mechanics, and this turns out to be true for problems in machine learning and optimization. Quantum algorithms beyond just linear algebra, with relevance for example to cryptography and to searching through huge datasets, also can be much more powerful than the best algorithms for classical hardware. I will show how to program quantum computers, with an emphasis on the hardware of IBM, Google, and D-Wave, then I will discuss the current state of quantum computing, including the difficulties and challenges.

Nike Dattani completed his undergraduate degrees in Mathematics, Physics and Biology at University of Waterloo, and a thesis with Ray Laflamme, Director at the Institute for Quantum Computing. He did his PhD in Chemistry at Oxford University in England, where he then became a Lecturer. He has also worked at the Harvard-Smithsonian Center for Astrophysics in USA, Kyoto University in Japan, Nanyang Technological University in Singapore, and been a Visiting Researcher at the Max Planck Institute for Solid State Research in Germany. He holds the record for the largest number factored using a quantum mechanical device (in this case an NMR-based quantum computer).