

Speakers

Susi Lehtola, University of Helsinki***Numerical methods for quantum chemistry***

Quantum chemistry has long been expected to be the "killer application" of quantum computers, which enable a native approach to electronic structure

calculations: the complicated interelectronic interactions involved in electronic structure are ideally suitable to be described with operations on quantum bits. However, even when large-scale quantum computers become available, the subproblem ideally solved on a quantum computer is only a small part in the larger flowchart required for an electronic structure calculation. In this talk, I will discuss ongoing work to improve the accuracy of the classical computing steps in quantum chemical calculations.

Dr Susi Lehtola received his PhD in theoretical physics at the University of Helsinki in 2013. Dr Lehtola did postdocs with Prof. Hannes Jónsson at Aalto University in 2013-2014 and with Prof. Martin Head-Gordon at Lawrence Berkeley National Laboratory in 2014-2017. Dr Lehtola was an Academy of Finland postdoctoral fellow at the Department of Chemistry of the University of Helsinki in 2017-2020, after which he worked as a Software Scientist at the Molecular Sciences Software Institute at Virginia Tech 2020-2022. Since 2022, Dr Lehtola is an Academy of Finland Research Fellow at the Department of Chemistry of the University of Helsinki. Dr Lehtola is well-known worldwide for his research in density functional theory, numerical methods, and reusable open source software for electronic structure theory.

Ulrich Fekl, University of Toronto**Quantum computers against classical computers: computations on a chemically important problem**

While we are still waiting for the universal quantum computer to become a reality, currently existing noisy intermediate scale quantum (NISQ) systems are being used for chemistry problems already. However, the selection of problems is often ad-hoc, a problem is rarely re-computed by another group, and how a chemical problem can be scaled to produce challenges of increasing difficulty, as NISQ machines grow bigger and more powerful, is not clear. We propose to use as a testbed the compound class of polymantanes, that is adamantane and its isomers, triamantane, tetramantane, etc. The smaller members of this class of molecules are computable with classical computers (ab initio and DFT), which provides an important benchmark for comparison. Also, polymantanes are stable and many are obtainable, such that experimental results can be consulted where needed. Lastly, polymantanes lead, in increments, to the structure of diamond, which, by virtue of being a solid-state material, presents a tremendous challenge for NISQ machines. Here we will present results on benchmarking NISQ-based computations (simulators and/or quantum hardware), using the variational quantum eigensolver (VQE) on adamantane and its isomers, compared to state-of-the art ab initio/composite accurate thermodynamics methods as well as DFT methods. Reaction barriers for interconversion of isomers are also computed classically and quantumly, for comparison.

Ulrich Fekl received his PhD in 2000 from the University of Erlangen-Nürnberg (Germany). His PhD, for experimental research on mechanisms of inorganic and organometallic reactions, was awarded “summa cum laude”. Studies included conventional and high-pressure conditions. In 2000 he moved to the University of Washington in Seattle (USA) to work with Professor Karen Goldberg on novel platinum(II) and platinum(IV) systems for alkane C-H bond activation. This work has been highly influential on the field and is highly cited. In 2003 he took up a faculty position at the University of

Toronto. Initial work was experimental, involving transition metal Lewis-acids to catalyze organic reactions and also reactions at coordinated ligands. Novel and useful reactions of dithiolene complexes were discovered. Ulrich Fekl received tenure at the University of Toronto in 2008. Experimental work in the group is increasingly being complemented by quantum chemistry. Aided by a recent collaboration (Jacobsen, U of T), we are particularly excited about exploring quantum computing for quantum chemistry.

Mikael Johansson, CSC

Entangling the power of supercomputing and quantum computing for chemistry



Classical supercomputers are immensely powerful, also for simulating chemical systems. This is due to two main reasons: the increase in computing power and method development. The latter is important to note. Extremely efficient approximations for studying quantum chemistry on binary calculators have now been advanced for almost a century. Schrödinger presented his wave equation in 1926, and already in 1927 Heitler and London studied the bonding within the hydrogen molecule. In order to gain quantum advantage as early as possible, a careful analysis of where that advantage is to be found is needed. Here, we will discuss the pain points for accurately and efficiently modelling chemistry on supercomputers, and explore how to make the most of quantum-accelerated high-performance computing.

Mikael Johansson is Manager for Quantum Technologies at CSC. He has twenty years of experience of studying and teaching quantum-mechanical methods and phenomena in chemical and biochemical systems in academia. In his present role, Johansson coordinates CSC's national and global efforts in quantum technologies, and in general explores and enables the uptake of quantum technologies.

Hannu Reittu, VTT



A new quantum community detection algorithm for reduction of molecular Hamiltonian matrices

So called Configuration-Interaction (CI) representation of many-electron problem of molecules uses exact quantum Hamiltonian of the corresponding electron system and a finite set of one-electron spin-orbitals. Such system of orbitals results in a finite dimensional Hilbert space in which a dimension corresponds to placing electrons in a set of orbitals forming so called Slater determinant. Hamiltonian operator is represented as a matrix in the basis of Slater determinants. To have a good accuracy, number of orbitals is much larger than number of electrons in a molecule. This circumstance results in many Slater determinants and large Hamiltonian matrix. The Hamiltonian matrix may be mapped to a weighted graph, in which nodes are Slater determinants and link weights are absolute values of the corresponding matrix elements of the Hamiltonian matrix. In a recent study, it was suggested to use graph-community detection to such a graph to find possible diagonal blocks of the Hamiltonian matrix. Such blocks are smaller than the original matrix but still can well represent spectral properties of the whole Hamiltonian matrix. A traditional community detection algorithm and its quantum implementation as a quadratic unconstrained binary optimization (QUBO) problem which can be solved on a quantum annealer or quantum gate computer using quantum approximate optimization algorithm (QAOA). We suggest another QUBO for solving the same problem which may be better suited for quantum computing. We also consider applications of reduced Hamiltonian in simulation of molecules on quantum computers. Aim is to reduce number of qubits needed. In a mainstream approach, using fermionic annihilation- creation operators, number of qubits is comparable to the number of Slater determinants. However, the Hamiltonian matrix is sparse due to so called Slater rules, most of the matrix elements are zeroes. This can be used to substantially reduce number of qubits needed. We suggest that the community based reduction of Hamiltonian matrix can further reduce the number of qubits.

Hannu Reittu is with VTT Technical Research Centre of Finland since 1998, where he currently works as Senior Scientist in Quantum algorithms and software team. He received Ph.D. in theoretical physics from Leningrad State University (now St. Petersburg State University) in 1990, and Ph.D. in physics from Wihuri Physical Laboratory at Turku University (Finland) in 1995. At VTT he has worked on stochastic modelling of networks, data analysis, machine learning and quantum algorithms. He has over 50 scientific publications listed in his Google Scholar account.

Hanna Linn, University of Chalmers***Resource analysis of quantum algorithms for coarse-grained protein folding models***

Protein folding processes are a complex and vital aspect of molecular biology that quantum devices may help model. We analyze the resource requirements for simulating protein folding on a quantum computer, assessing this problem's feasibility in the current and near-future technological landscape. We calculate the minimum number of qubits, interactions, and two-qubit gates necessary to represent the energy of a specific folding. We study coarse-grained folding models on the lattice and the fixed backbone side-chain conformation model and assess these models' compatibility with the constraints of existing quantum hardware given different bit-encodings. Specifically, we focus on the resources needed to encode the Hamiltonian representing the energy function of each protein folding model concerning the chain's amino acid count. The energy Hamiltonian is a fundamental component of the chosen quantum algorithm and guides the evolution of the quantum state for efficient computations. We conclude that the number of qubits required falls within current technological capabilities. Further, the limiting factor is the high number of terms in the Hamiltonian, resulting in a substantial requirement for numerous quantum gates not available today.

Hanna Linn is a PhD student at Chalmers University of Technology and Wallenberg Center of Quantum Technology (WACQT) with supervisors Göran Johansson and Laura García Álvarez. Her primary research is in the field of quantum algorithms within life science, and the latest project has been on protein folding with classical quantum hybrid algorithms. She did her Bachelor's in Engineering Physics and my Master's in Machine Learning at the Royal Institute of Technology in Stockholm.

Jose Lado, Aalto University***Emulating noisy quantum algorithms with tensor-networks***

Understanding the performance of quantum algorithms in the presence of noise for large quantum circuits goes well beyond the capabilities of conventional quantum circuit simulators. Here, we show that a quantum many-body-inspired simulation of quantum circuits based on tensor networks allows us to emulate large, noisy quantum circuits with classical computational resources. We discuss the intimate relation between the tensor-network complexity and the qubit and gate fidelities, analyzing the bounds in the quantum circuit entanglement. We analyze the feasibility of several algorithms as a function of the effective noise in large quantum circuits, and we map out the entanglement that is generated during the execution of these algorithms. We find that a variety of algorithms can provide faithful results even at a moderate loss of entanglement. Focusing on a quantum circuit designed to compute topological invariants in quantum materials, we show the capability of such an algorithm to provide faithful results for moderately noisy quantum circuits. Our results show that tensor-network approaches offer a powerful platform to benchmark quantum algorithms in large quantum circuits, allowing us to establish which algorithms can provide faithful results in large, near-term noisy quantum circuits.

Jose Lado is an assistant professor in theoretical physics at Aalto University in Finland since 2019, where he leads the Correlated Quantum Materials group. He was an ETH Fellow at the Institute for Theoretical Physics at ETH Zurich in Switzerland between 2017-2019, and he got his Ph.D. working at INL in Portugal between 2013-2016. His research focuses on the design of quantum materials featuring exotic quantum properties at macroscopic scales driven by topology and correlations. His group develops a variety of quantum many-body methods to engineering correlated quantum

matter, and he often collaborates with experimental groups designing quantum materials. He has authored more than 90 scientific publications, and he has given more than 30 invited talks since 2019.

Gopal Peddinti, VTT

Potential for applying quantum computing in synthetic biology

Synthetic biology studies often constitute a variety of computational modelling along with biological big data. We currently focus on identifying computational problems in synthetic biology that may benefit from the use of quantum computing. Quantum computing may potentially be used in solving several computational biology problems, including de novo sequence assembly, de novo protein design, genome-scale metabolic model optimization, and enzyme property predictions using molecular simulations (e.g., QM/MM modelling). However, quantifying the gains in terms of computational efficiency or performance, is still subject to further research.

Gopal Peddinti acquired an M.Sc. in pure mathematics from the University of Hyderabad (India) in 2001, followed by an M.Tech. in computer science from the Indian Institute of Technology Kharagpur (India) in 2003. Subsequently, he obtained his Ph.D. in bioinformatics and computational systems biology from Aalto University (Finland) in 2010. Currently, serving as a senior scientist within VTT's Bioanalytics and Biological Data Science team, his primary research centers on computational biology applications in industrial biotechnology.

Rupesh More, Neste

QC challenges and opportunities in Chemical R&D

