APPLICATION OF JÜLICH UNIVERSAL QUANTUM COMPUTER SIMULATOR

FINDING GROUND-STATE OF THE HUBBARD MODEL USING QUANTUM ANNEALING

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Quantum computing

... promises to solve some of our toughest problems

Drug design

Materials design

Supply chain logistics

Traffic optimization

Energy grid management

Vegetation evolution – climate change

Human brain functionality – neural networks

Quantum computing

Quantum states

- Fundamental unit $\rightarrow$ qubit $\rightarrow$ $|0\rangle$ or $|1\rangle$?

- A general state of a single qubit can be written as,

$$|q_1\rangle = a_0|0\rangle + a_1|1\rangle$$

- A general state of n qubits can be written as,

$$\begin{aligned}|q_n\rangle &= a_{0\ldots 0}|0\ldots 0\rangle + a_{0\ldots 1}|0\ldots 1\rangle + \ldots + a_{1\ldots 1}|1\ldots 1\rangle \\ &= a_0|0\rangle + a_1|1\rangle + \ldots + a_{2^n-1}|2^n - 1\rangle\end{aligned}$$

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Quantum computing

Quantum gates

- An example of a universal set of quantum gates is,

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},\ T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix},\ CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

- Transformation of states in quantum computing is **unitary.**

- Unitary transformations can be decomposed into sequences of single and two qubit gates.

Quantum algorithms

Some examples:

1. Shor’s algorithm for factorization
2. Grover’s search algorithm
3. Variational quantum algorithms
4. **Quantum annealing**

These quantum algorithms can be implemented on a gate-based quantum computer using a specific sequence of the universal gates, also called a **quantum circuit**.

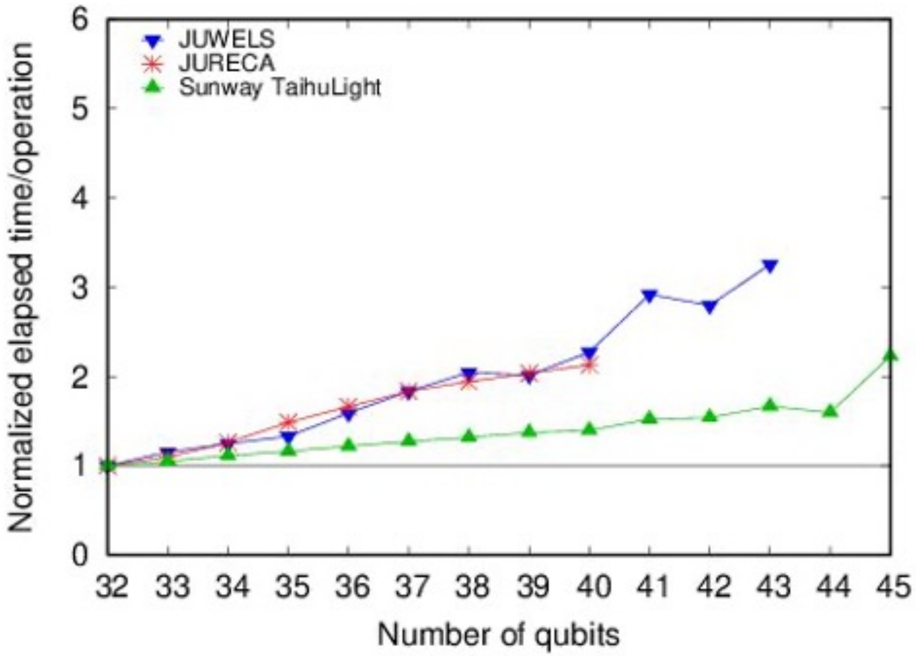
Important to develop software to investigate the performance of quantum algorithms.

JUQCS

Jülich Universal Quantum Computer Simulator

- High-performance software for simulating a gate-based quantum computer.
- Uses **storage of only 2^n complex scalars** to faithfully simulate an n-qubit quantum computer: n qubits $\rightarrow 2^n \times 16$ bytes of memory.

Simulates up to 42-qubits using 512 nodes of JUWELS-Booster.
Will simulate up to 47-qubits using 4096 nodes of JUPITER.



H. De Raedt et al., Computer Physics Communications 237 (2019) 47–61

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Application

Finding ground-state of the Hubbard model

- In 1-dimension, the model Hamiltonian takes the form:

$$H_H = -\frac{t}{2}\sum_{\substack{i=1\\ i\neq L}}^{2L-1}(X_iX_{i+1}+Y_iY_{i+1}) + \frac{u}{4}\sum_{i=1}^{L}(I-Z_i)(I-Z_{i+L})$$

  where X_i, Y_i, Z_i are Pauli matrices acting on qubit i.

- The problem is to solve the eigenvalue equation,

$$H_H|\phi\rangle = E|\phi\rangle$$

  to find the lowest eigenvalue E_0 and the corresponding eigenstate $|\phi_0\rangle$.

  - Exact diagonalization: $O(2^{6L})$
  - …
  - Bethe ansatz: $O(L^p)$

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Quantum annealing

- We can implement quantum annealing on a gate-based quantum computer to find the ground-state.
- The annealing Hamiltonian that we choose:

$$H(s) = -\frac{t}{2}\sum_{\substack{i=1\\ i\neq L}}^{2L-1}(X_iX_{i+1}+Y_iY_{i+1}) + \frac{su}{4}\sum_{i=1}^{L}(I-Z_i)(I-Z_{i+L})$$

- The state is obtained by solving the time-dependent Schrödinger equation

$$i\frac{d}{dt}|q_{2L}(t)\rangle = H(t)|q_{2L}(t)\rangle$$

the solution of which can be calculated by

$$|q_{2L}(T_A)\rangle = U(T_A)|q_{2L}(0)\rangle$$

where T_A is the annealing time and $U(T_A)$ is constructed using the second order Suzuki-Trotter product-formula algorithm.

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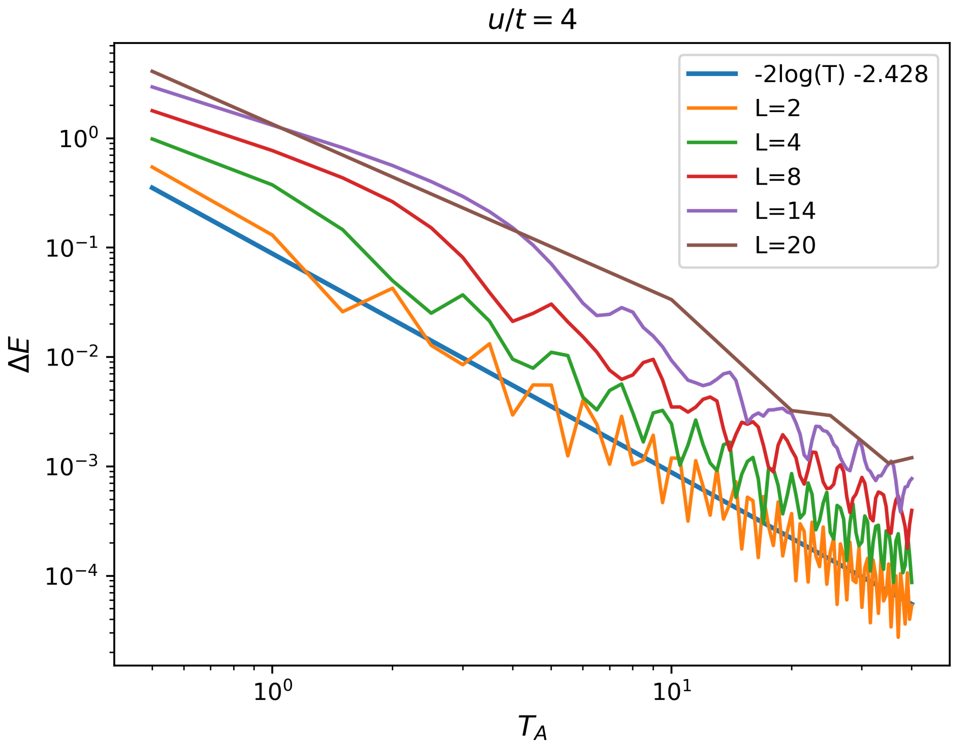
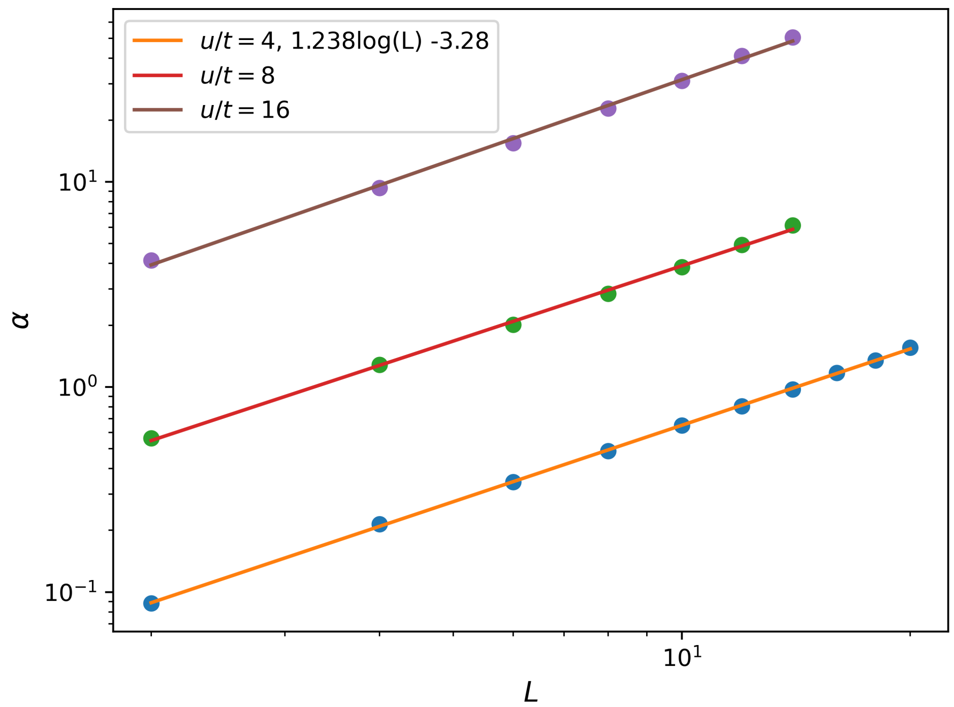
Results

- After constructing circuits for $U(T_A)$ for a range of L and T_A, we simulate them using JUQCS.
- Energy of the state $|q_{2L}(T_A)\rangle$: $\langle q_{2L}(T_A)|H_H|q_{2L}(T_A)\rangle$.
- Energy residue: $\langle q_{2L}(T_A)|H_H|q_{2L}(T_A)\rangle - E_0$.





$$\Delta E = \frac{\alpha(L)}{T_A^2} \quad \rightarrow \quad T_A \propto \frac{L^{0.62}}{\Delta E} \quad \leftarrow \quad \alpha(L) \propto L^{1.238}$$

Summary

- The arena of high performance simulations can thus go a long way in informing us about the utility of quantum algorithms even before the emergence of real hardware to test them.

- The time required to find a reasonable estimate of the ground-state of the 1-dimensional Hubbard model for quantum annealing scales sub-linearly with system size.

- The time complexity of $O(L^{0.62})$ suggests a quantum speed-up over classical methods to find the ground-state.

Thank you very much!