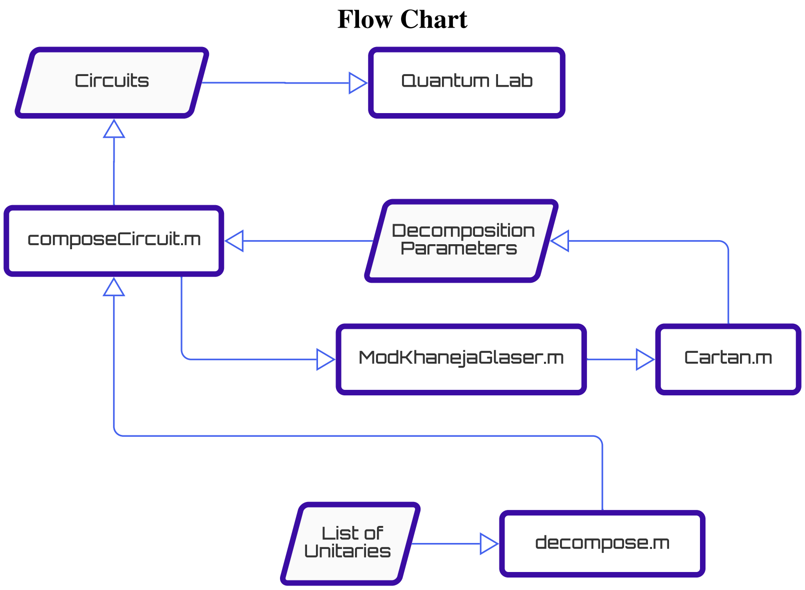
Supplementary Note 1

Algorithm



Supplementary Figure 1. Flow chart of the algorithms used to go from the Hamiltonian to a list of circuits implementing the evolution. This can be started from the list of unitaries directly if these are available instead of starting from a Hamiltonian. Final result (top) is a python script which can be compiled using *Qiskit* to build the circuits.

Supplementary Figure 1 summarises the workflow of operations that make up our simulation algorithm. All scripts are written in the MATLAB programming language, the natural language when dealing with matrix manipulations.

The core of the software is the *decompose.m* function, which calls takes as input a list of 8x8 unitary matrices and returns a string giving the quantum circuit in a format understandable by *Qiskit*. To compile, the contents of the string must be copied into the Quantum Lab available in IBM Q Experience.

The most important part of the algorithm lies in the function computing the Cartan decomposition of a unitary, available through *Cartan.m*. This takes as arguments a unitary and the 3 subspaces that define the decomposition. A subspace is defined by a list of matrices which form an orthogonal basis under the inner product of $\mathfrak{su}(2^n)$. All subspaces necessary for the decomposition of $\mathfrak{su}(4)$ and $\mathfrak{su}(8)$ are available as global variables through the script *suGen.m*. The code for the implementation is available as separate Supplementary Data.

Supplementary Note 2

Calibrations and additional data

The official calibration data for the quantum computers used to perform the simulations is available in Supplementary Table 1 and Supplementary Table 2. Data taken with the older generation ibmqx2 is available in Supplementary Figure 2.

Qubit	T1 (µs)	T2(µs)	Readout error	1Q gate error	CNOT error
Q0	111.74	103.88	2.42%	0.28‰	0->1: 9.5‰
Q1	125.9	12.19	1.17%	0.89‰	1->2: 9.4‰
Q2	159.84	95.24	6.81%	0.20‰	2->3: 7.0‰
Q3	186.01	84.16	1.51%	0.23‰	3->4: 7.1‰
Q4	124.12	148.87	3.76%	0.32‰	-

Supplementary Table 1. Calibration data for *ibmq_santiago* from 06.11.2020. T1 and T2 are the relaxation times of the qubit. The readout error represents the infidelity of the measured statistics with respect to the real statistics. The last two columns quantify the average infidelities of the respective operations due to imperfect control.

Qubit	T1 (μs)	T2(μs)	Readout error	1Q gate error	CNOT error
Q0	56.25	26.87	6.31%	2.15‰	0->1: 27.6‰, 0->2: 16.1‰
Q1	46.98	21.22	7.92%	1.72‰	1->2: 20.7‰
Q2	61.67	90.25	3.46%	0.46‰	2->3: 12.5‰, 2->4: 12.5‰
Q3	60.97	30.58	1.31%	0.47‰	3->4: 15.7‰
Q4	72.81	29.98	3.83%	0.66‰	-

Supplementary Table 2. Calibration data for *ibmqx*2 from 06.11.2020. T1 and T2 are the relaxation times of the qubit. The readout error represents the infidelity of the measured statistics with respect to the real statistics. The last two columns quantify the average infidelities of the respective operations due to imperfect control.

Site		1	2	3	4	5	6	7	8
FMO	Raw	0.724	0.207	0.0628	0.0688	0.1114	0.205	0.0645	0.525
	Mitigated	0.550	0.198	0.0203	0.0393	0.1077	0.186	0.0296	0
Linear Chain	Raw	0.1389	0.0727	0.0669	0.666	0.689	0.0846	0.1458	0.0530
	Mitigated	0.0645	0.0343	0.0458	0.0517	0.0421	0.0521	0.0764	0

Supplementary Table 3. Computed accuracy errors A for different sets of data. We see that the deviation of the data from the simulation is lowered by the mitigation process for all sites. Higher inaccuracies are observed in simulating the FMO than the linear chain.

Supplementary Note 3

Accuracy

As a result of gaussian errors in controlling the gate parameters in the physical device we observe a decrease in the expected signal at readout and an overlapped level of noise which appears constant for all unitaries and all sites. To compare the quality of the raw data against the mitigated data in predicting the value of the simulated populations we devise a metric that only accounts for accuracy. Let y_n be N random variables assumed of the form

$$y_n = g(x_n) + \bar{y}_n, \tag{1}$$

where $\bar{y}_n$ are gaussian random variables of mean 0 and standard deviation σ_n. We quantify the degree to which the function g approximates f by the average square distance

$$A^2 = \frac{1}{N}\sum_n (g(x_n) - f(x_n))^2. \tag{2}$$

Since we only have access to the data points y_n, and not the averages we look at the function

$$J = \frac{1}{N}\sum_n (y_n - f(x_n))^2 \tag{3}$$

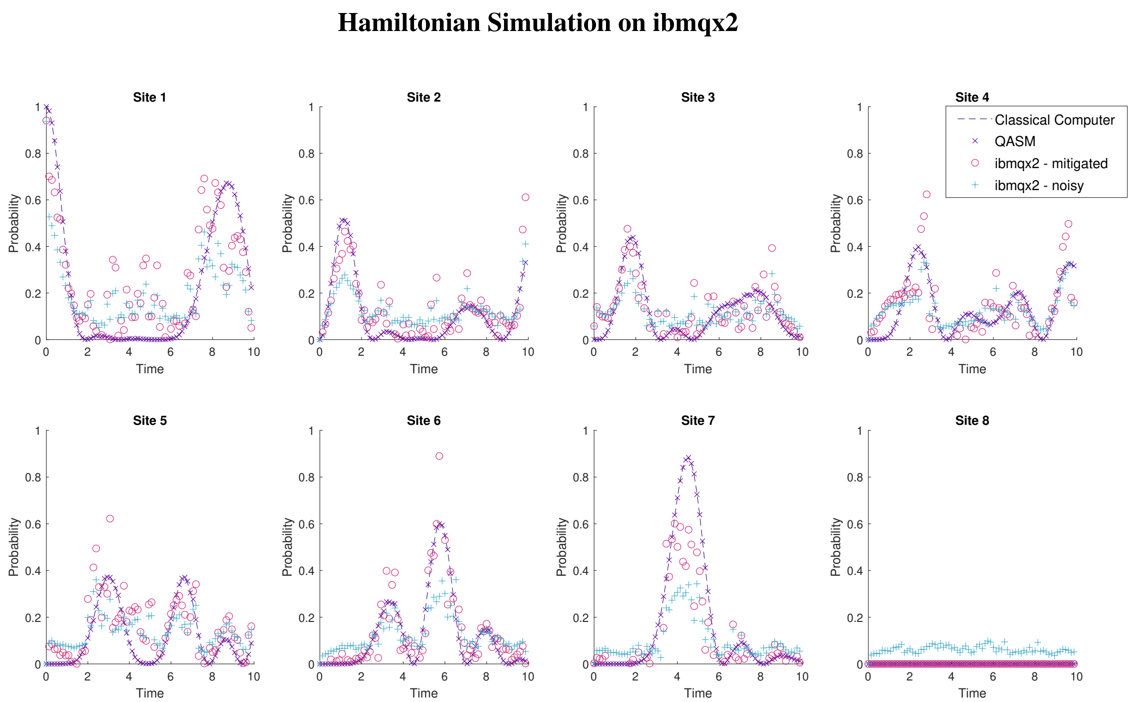
As the number of data points grows we expect J to approach its mean value

$$< J >= \frac{1}{N}\sum_n [(g(x_n) - f(x_n))^2 + < \bar{y}_n^2 >] = \frac{1}{N}\sum_n [(g(x_n) - f(x_n))^2 + \sigma_n^2]. \tag{4}$$

Using this we can express the metric A in terms of the data points

$$A^2 = J - \frac{1}{N}\sum_n \sigma_n^2. \tag{5}$$

We compute this for all sites in the case of both the FMO and the linear ordered chain, using both the raw and the mitigated data. The results can be seen in Supplementary Table 3.



Supplementary Figure 2. Simulation of the linear chain Hamiltonian on the old generation QV 8 ibmqx2. Mitigation proves less effective due to large statistical errors, as observed in the population of site 8. Despite having better connectivity, the low quality of the qubits involved leads to numerous systematic errors. Interestingly, the artefact in the middle of site 1 does not vanish even in this quantum device.