quantum-accelerated scientific computing: concepts, programming tools and applications

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collaborations, funding and support



quantum computing in the news

Article

Quantum supremacy using a programmable superconducting processor

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On "Quantum Supremacy"



October 21, 2019 Written by: Edwin Pednault, John Gunnels & Dmitri Maslov, and Jay Gambetta

Recent advances in quantum computing have resulted in two 53-qubit processors: one from our group in IBM and a device described by Google in a paper published in the journal *Nature*. In the paper, it is argued that their device reached "quantum supremacy" and that "a state-of-the-art supercomputer would require approximately 10,000 years to perform the equivalent task." *We argue that an ideal simulation of the same task can be performed on a classical system in 2.5 days and with far greater fidelity*. This is in fact a conservative, worst-case estimate, and we expect that with additional refinements the classical cost of the simulation can be further reduced.

quantum computing in Europe



Computertechnologie

Ein Quantensprung für Deutschland?

Stand: 15.06.2021 18:25 Uhr

In Ehningen bei Stuttgart wurde Europas erster Quantencomputer eingeweiht. Der ultraschnelle Rechner der Firma IBM soll der Wirtschaft helfen, im Wettstreit mit China und den USA zu bestehen.

TECHNOLOGY NEWS MAY 11, 2021 / 10:52 AM / UPDATED 5 MONTHS AGO

Germany to support quantum computing with 2 billion euros

By Reuters Staff

2 MIN READ

FOCUS AREAS

S AREAS COLLABORATION OUR IMPACT ABOUT TNO CAREER

THE FIRST EUROPEAN ONLINE QUANTUM COMPUTER PLATFORM

4 May 2020 • 3 min reading time

Leading universities and quantum huse from China to America and the Netherlands are working on the development of a usable quantum computer. Within QuTech, TNO is working on innovative quantum technology in collaboration with Delft University of Technology and with some success, because a new version of the 'Quantum Inspire' quantum computing platform was launched on 20 April 2020. It is, in fact, the first European quantum computer platform that is generally accessible online.

09.04.2021 . Awards

Quantum Delta NL awarded 615 million euro from Netherlands' National Growth Fund to accelerate quantum technology



quantum-accelerated scientific computing

- concepts
 - qubits, gates, and simple algorithms
- programming tools
 - LibKet and generation of resource-optimal quantum circuits

applications

- quantum linear solvers and optimization algorithms
- summary

concepts

qubits, gates, and simple algorithms

von Neumann model



int a = 1; int b = 2; int c = a+b;



von Neumann model



а	=	1;
b	=	2;
С	=	a+b;
	a b c	a = b = c =

ld r0 mem(a)
ld r1 mem(b)
add r0 r1 r2
sd r2 mem(c)



a quantum computer model





2-qubit gates between nonadjacent qubits require additional 'swap' ops

quantum bits

• **qubit**: quantum version of a bit

 $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle, \qquad \alpha, \beta \in \mathbb{C}, \qquad |\alpha|^2 + |\beta|^2 = 1$

computational basis

$$\mathcal{E} = (|0\rangle, |1\rangle) = \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right)$$

coefficients α, β are the probability amplitues and |α|² and |β|² are the probabilities of measuring the basis states |0⟩ and |1⟩, respectively

single-qubit states

Bloch sphere

$$|\psi\rangle = \frac{\partial \psi}{\partial t} \left(\cos \frac{\theta}{2} |0\rangle + e^{i\varphi} \sin \frac{\theta}{2} |1\rangle \right)$$

- polar angle $\theta \in [0, \pi]$
- azimutal angle $\varphi \in [0, 2\pi)$
- global phase δ



quantum gates

Pauli X

Hadamard



$$-H - \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

- unitary operations represented by unitary matrices
- all quantum gates are reversible, e.g. $HH^{\dagger} = I$

single-qubit gates



single-qubit gates



single-qubit circuits

$$|\psi_{\scriptscriptstyle in}
angle - U_1 - U_2 - U_3 - |\psi_{\scriptscriptstyle out}
angle$$

• single-qubit gates U_k are **unitary matrices**, i.e.

$$U_k U_k^{\dagger} = U_k^{\dagger} U_k = I$$

quantum circuits are sequences of matrix-vector multiplications

$$|\psi_{out}\rangle = U_3 U_2 U_1 |\psi_{in}\rangle$$

multi-qubit states

$$|\psi_0\rangle = \alpha_0 |0\rangle + \beta_0 |1\rangle = \alpha_0 \begin{pmatrix} 1\\0 \end{pmatrix} + \beta_0 \begin{pmatrix} 0\\1 \end{pmatrix}$$
 tensor product
$$|\psi_1\rangle = \alpha_1 |0\rangle + \beta_1 |1\rangle = \alpha_1 \begin{pmatrix} 1\\0 \end{pmatrix} + \beta_1 \begin{pmatrix} 0\\1 \end{pmatrix}$$
 $|A\rangle \otimes |B\rangle = \begin{bmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{bmatrix}$

tensor product of two single-qubit states

 $|\psi_0\rangle \otimes |\psi_1\rangle = \alpha_0 \alpha_1 |00\rangle + \alpha_0 \beta_1 |01\rangle + \beta_0 \alpha_1 |10\rangle + \beta_0 \beta_1 |11\rangle =: |\psi_0 \psi_1\rangle$

with

$$|\alpha_0 \alpha_1|^2 + |\alpha_0 \beta_1|^2 + |\beta_0 \alpha_1|^2 + |\beta_0 \beta_1|^2 = 1$$

multi-qubit states

tensor product of n single-qubit states

 $|\psi_0 \dots \psi_n\rangle = \gamma_{0\dots 00} |0 \dots 00\rangle + \gamma_{0\dots 01} |0 \dots 01\rangle + \dots + \gamma_{1\dots 11} |1 \dots 11\rangle$

• an *n*-qubit register can hold the 2^n inputs 'simultaneously' in **superposition**

a few words of caution

- it is impossible to obtain the γ 's; one obtains a single binary answer, say, $|001101\rangle$ with probability $|\gamma_{001101}|^2$ upon **measurement**
- a single run of a quantum circuit is not very useful; many runs are required to measure the correct answer with sufficient certainty

example: 3-bit password



Grover's algorithm

quantum circuit on QI



quantum circuit on IBM





multi-qubit gates



$$H \otimes I|00\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & 1\\ 1 & 0 & -1 & 0\\ 0 & 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0\\ 0\\ 0\\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0\\ 1\\ 0 \end{pmatrix} = \frac{|00\rangle + |10\rangle}{\sqrt{2}} = \frac{(|0\rangle + |1\rangle) \otimes |0\rangle}{\sqrt{2}}$$

entanglement

$$CNOT(H \otimes I)|00\rangle = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\ 0\\ 1\\ 0 \end{pmatrix} = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

 Bell state is maximally entangled. By measuring one of the two qubits one knows the value of the other qubit without a further measurement



programming tools

LibKet and generation of resource-optimal quantum circuits

Lib – The **k**wantum **e**xpression **t**emplate **Lib**rary





quantum acceleration workflow



quantum acceleration workflow



different programming philosophies

standard quantum SDKs

apply gates to individual qubits

```
H q[0:2]
X q[0,2]
H q[2]
CCX q[0], q[1], q[2]
```

...



LibKet

'stream' qubits through gates

```
...CCX(q[0],
 q[1],
 q[2](
 H(q[2](
 X(q[0,2](
 H(q[0:2]())
 ))
 ))
))
```

different programming philosophies

standard quantum SDKs

apply gates to individual qubits

```
H q[4,7,8]
X q[4,8]
H q[8]
CCX q[4], q[7], q[8]
```

...

	init grover(1)							
q[4]	-H-X	•	X H	X	•	X-H-7		
 q[7]	H	•	H	X	•	-X-H-7		
q[8]	-H-X-H	- 6 -H-	-X-H-	-X-H-	<u>о</u> -н	-X-H-?		

LibKet

'stream' qubits through gates

```
...CCX(q[0],
    q[1],
    q[2](
    H(q[2](
        X(q[0,2](
            H(q[0:2](q[4,7,8]))
        ))
    ))
    ))
```

selective 'views' on the qubits

auto f0 = select<0,2,3>();



selective 'views' on the qubits

auto f0 = select<0,2,3>(); auto f1 = range<1,2>(f0);



```
auto f0 = select<0,2,3>();
auto f1 = range<1,2>(f0);
auto f2 = tag<0>(f1);
```



```
auto f0 = select<0,2,3>();
auto f1 = range<1,2>(f0);
auto f2 = tag<0>(f1);
auto f3 = qubit<1>(f2);
```





```
auto f0 = select<0,2,3>();
auto f1 = range<1,2>(f0);
auto f2 = tag<0>(f1);
auto f3 = qubit<1>(f2);
auto f4 = tag<1>(f3);
```



```
auto f0 = select<0,2,3>();
auto f1 = range<1,2>(f0);
auto f2 = tag<0>(f1);
auto f3 = qubit<1>(f2);
auto f4 = tag<1>(f3);
auto f5 = gototag<0>(f4);
```



```
auto f0 = select<0,2,3>();
auto f1 = range<1,2>(f0);
auto f2 = tag<0>(f1);
auto f3 = qubit<1>(f2);
auto f4 = tag<1>(f3);
auto f5 = gototag<0>(f4);
auto f6 = gototag<1>(f5);
```



```
auto e0 = init();
```



```
auto e0 = init();
auto e1 = sel<0,2>(e0);
```



```
auto e0 = init();
auto e1 = sel<0,2>(e0);
auto e2 = h(e1);
```



```
auto e0 = init();
auto e1 = sel<0,2>(e0);
auto e2 = h(e1);
auto e3 = all(e2);
```







3-qubit Grover's algorithm

```
auto expr = measure(diffusion(oracle(h(init())));
QDevice<backend, 3> device;
utils::json res = device(expr).eval(shots);
cout << device.get<QResultType::best>(res) << endl;</pre>
```



3-qubit Grover's algorithm

- IBM's basis gates: CX, ID, RZ, SX, X
- executable quantum circuit generated by IBM's quantum compiler



```
auto expr = measure(diffusion(oracle(h(init())));
QDevice<QDeviceType::ibmq_quito, 3> device;
utils::json res = device(expr).eval(shots);
cout << device.get<QResultType::best>(res) << endl;</pre>
```



traditional quantum circuit compilation

gate substitution rules

$$H \to R_x(\pi)R_y(\pi/2), \qquad H \to R_y(-\pi/2)R_x(\pi), \qquad \dots$$

cancelling of inverse gates

$$CZ CZ^{\dagger} = I, \qquad R_{\chi}(\theta)R_{\chi}(-\theta) = I, \qquad \dots$$

aggregation using commutativity or fusion rules

 $HR_{z}(\theta)H = R_{x}(\theta), \theta \in \{\pi, \pm \pi/2\}, \qquad R_{z}(\theta_{1})R_{z}(\theta_{2}) = R_{z}(\theta_{1} + \theta_{2}), \qquad \dots$

approximate computing

• our aim is to generate a resource-efficient directly executable circuit $U(\theta)$ that mimics the expectation-value behavior of the textbook circuit V



approximate computing

• our aim is to generate a resource-efficient directly executable circuit $U(\theta)$ that mimics the expectation-value behavior of the textbook circuit V



approximate computing

$$U_{\text{opt}} = \underset{U \in \mathcal{U}_s}{\operatorname{argmin}} \min_{\boldsymbol{\theta}_U} \max_{|\psi\rangle \in \Psi} F(|\psi\rangle; V, U(\boldsymbol{\theta}_U)), \quad s \to \min$$

cost function

$$F(|\psi\rangle; V, U(\theta_U)) = \sum_{k} \left(\langle A^k \rangle_{V|\psi\rangle} - \langle A^k \rangle_{U(\theta_U)|\psi\rangle} \right)$$

- A^k is an observable, e.g., Pauli-X, Y, Z gate
- expectation value of state $|\psi\rangle$ upon application of operator P

$$\left\langle A^{k}\right\rangle _{P\left|\psi\right\rangle }=\left\langle (P\psi)^{\dagger}\left|A^{k}\right|P\psi\right\rangle$$

- U_s is the set of all admissible quantum circuits of size s
- $U(\boldsymbol{\theta}_U)$ is one parametrized quantum circuit with $\boldsymbol{\theta}_U = (\theta_1, \dots, \theta_N)^{\top}$

selected results



algo	#qubits	rigetti	ours		ibm		ours	
2q qft	2	18	16	11%	12-42	11	8-73%	
3q qft	5	118	92	22%	57-73	56	1-23%	
ccnot	3	33	15	54%	18	10	44%	
4q add	8	197	132	33%	116-131	74	36-43%	
8q add	16	474	312	34%	272-299	174	36-42%	
mc3x	4	90	76	15%	46-102	36	21-64%	
mc4x	5	195	164	16%	94-150	76	23-49%	
2q grover	2	15	8	46%	16-27	8	50-71%	
bv	4	21	11	47%	22	11	50%	

S. Adarsh, M. Möller: Resource Optimal Executable Quantum Circuit Generation Using Approximate Computing. To appear the Proceedings of IEEE International Conference on Quantum Computing and Engineering (QCE21), 2021.



selected results

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applications

quantum linear solvers and optimization algorithms

potential quantum applications

 $\min_{\theta} x_{\theta}^{\dagger} M_{\theta} x_{\theta}$ s. t. $A_{\theta} x_{\theta} = b_{\theta}$

HHL-type quantum linear solver

Find $x^{\dagger}Mx$ s.t. Ax = b

sparse matrices 0(left)

 $O(\log(N)\kappa^2/\epsilon)$ polylog(1/ ϵ)

• dense matrices $O(\sqrt{N}\log(N)\kappa^2/\epsilon)$

[Harrow, Hassidim, Lloyd 2009] [Childs, Kothari, Somma 2017]

[Wossnig et al. 2018]

applications

- linear differential equations [Berry 2010, Xin et al. 2018]
- nonlinear differential equations [Leyton, Osborne 2008, Liu et al. 2021]
- Poisson equation [Cao et al. 2013, Montanaro 2015]
- principal component analysis [Lloyd et al. 2014]
- data fitting [Wiebe et al. 2012]
- machine learning [Lloyd et al. 2013, Adcock et al. 2015, Biamonte et al. 2017, Schuld et al. 2018, Perdomo-Ortiz et al. 2018, …]

caveats



- you don't get the solution vector x but a scalar value x[†]Mx
- circuits are impractical for nearfuture quantum computers
- Recent step-by-step HHL algorithm walkthrough by Morrell and Wong (08/2021):

"[...] due to the imperfection and noise in a real quantum computer (ibmq_santiago), the hardware execution of the same circuit (for a 2x2 matrix) does not give satisfactory result" arXiv:2108.09004



E. Cappanera: Variational quantum linear solver for finite element problems, Master Thesis TU Delft, 2021.



HHL simulation with Qiskit: 2x2 matrices, w/o noise





HHL simulation with Qiskit: 2x2 matrices, with noise



S. Sigurdsson: Implementations of quantum algorithms for solving linear systems, Master Thesis TU Delft, 2021.



HHL simulation with Qiskit: 4x4 matrices, w/o noise



HHL simulation with Qiskit: 4x4 matrices, with noise

HHL simulation with Qiskit: 8x8 matrices, w/o noise

HHL simulation with Qiskit: 8x8 matrices, with noise

potential near-future quantum applications in SciComp

hybrid quantum-classical algorithms

- quantum approximate optimization algorithm (QAOA) [Farhi et al. 2014]
- quantum alternating operator ansatz (QAOA) [Hadfield et al. 2017]
- variational quantum eigensolver (VQE) [Peruzzo et al. 2014]
- variational quantum linear solver (VQLS) for sparse matrices [Bravo-Prieto et al. 2019 & Xu et al. 2019]

QAOA workflow

M. Alam, A. Ash-Saki, S. Ghosh: Analysis of quantum approximate optimization algorithm under realistic noise in superconducting qubits. arXiv: 1907.09631 (2019)

truss structure optimization

3-truss structure

options: $2^{\#trusses \times \#areas} = 512$

valid options

Option	q_0	q_1	q_2	q_3	q_4	q_5	q_6	q_7	q_8
1	0	0	1	0	0	1	0	0	1
2	0	0	1	0	0	1	0	1	0
3	0	0	1	0	0	1	1	0	0
4	0	0	1	0	1	0	0	0	1
5	0	0	1	0	1	0	0	1	0
6	0	0	1	0	1	0	1	0	0
7	0	0	1	1	0	0	0	0	1
8	0	0	1	1	0	0	0	1	0
9	0	0	1	1	0	0	1	0	0
10	0	1	0	0	0	1	0	0	1
11	0	1	0	0	0	1	0	1	0
12	0	1	0	0	0	1	1	0	0
13	0	1	0	0	1	0	0	0	1
14	0	1	0	0	1	0	0	1	0
15	0	1	0	0	1	0	1	0	0
16	0	1	0	1	0	0	0	0	1
17	0	1	0	1	0	0	0	1	0
18	0	1	0	1	0	0	1	0	0
19	1	0	0	0	0	1	0	0	1
20	1	0	0	0	0	1	0	1	0
21	1	0	0	0	0	1	1	0	0
22	1	0	0	0	1	0	0	0	1
23	1	0	0	0	1	0	0	1	0
24	1	0	0	0	1	0	1	0	0
25	1	0	0	1	0	0	0	0	1
26	1	0	0	1	0	0	0	1	0
27	1	0	0	1	0	0	1	0	0

invalid options

485

J. De Zoete: A practical quantum algorithm for solving structural optimization problems. Master Thesis, TU Delft, 2021.

preliminary results using Rigetti's simulator

J. De Zoete: A practical quantum algorithm for solving structural optimization problems. Master Thesis, TU Delft, 2021.

preliminary results using Rigetti's Aspen-9 processor

only 9 out of 64 options are valid and the exclusion criterion is sensitive to noise

J. De Zoete: A practical quantum algorithm for solving structural optimization problems. Master Thesis, TU Delft, 2021.

summary

- QC is not just for physicists and electrical engineers but should interest the entire CSE community as a potential future accelerator technology
- building quantum computers is just the beginning, the time has come to develop practical algorithms and software for solving real-world problems
- early experience with quantum-accelerated applications will hopefully guide QC vendors in the development of practically usable devices for end-users

Thank you for your attention and enjoy your dinner!