Quantum-accelerated scientific computing finally made easy

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Joint work with Tim Driebergen, Merel Schalkers, Kelvin Loh, and Richard Versluis

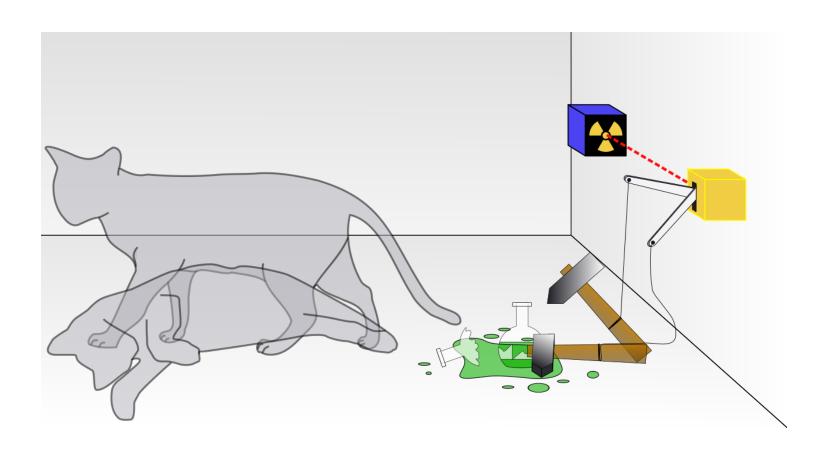
Outlook

- Basic concepts of quantum computing
 - Single- and multi-qubit states, gates, and simple algorithms
- Quantum-accelerated scientific computing
 - NISQ devices, programming models, and potential algorithms
- LibKet
 - Design principles and ongoing applications development
- Conclusion

Basic concepts of quantum computing

QUANTUM BITS AND GATES

Schrödinger's cat



Schrödinger's cat, cont'd

Before opening the box:
 superposition of two states



After opening the box:
 collapse to a single state



- Further examples of two-state quantum-mechanical system
 - spin of an electron (up, down)
 - polarization of a photon (vertical, horizontal)

Quantum bits

Qubit: basic unit of quantum information (quantum version of a bit)

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

Computational basis

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

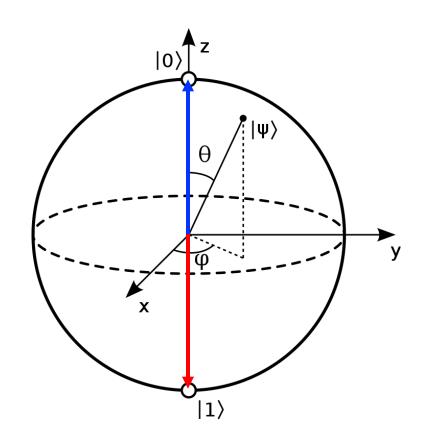
• Coefficients α , β are the **probability amplitues** and $|\alpha|^2$ and $|\beta|^2$ are the **probabilities** of measuring the basis states $|0\rangle$ and $|1\rangle$, respectively

Single-qubit states

Bloch sphere

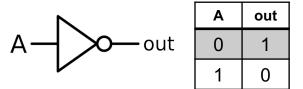
$$|\psi\rangle = e^{i\theta} \left(\cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle\right)$$

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

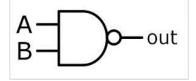


Classical gates

NOT



NAND

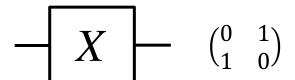


Α	В	out
0	0	1
0	1	1
1	0	1
1	1	0

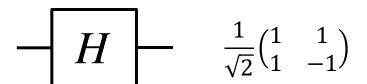
- Logical operations based on truth tables
- Most classical gates are not reversible

Quantum gates

Pauli X

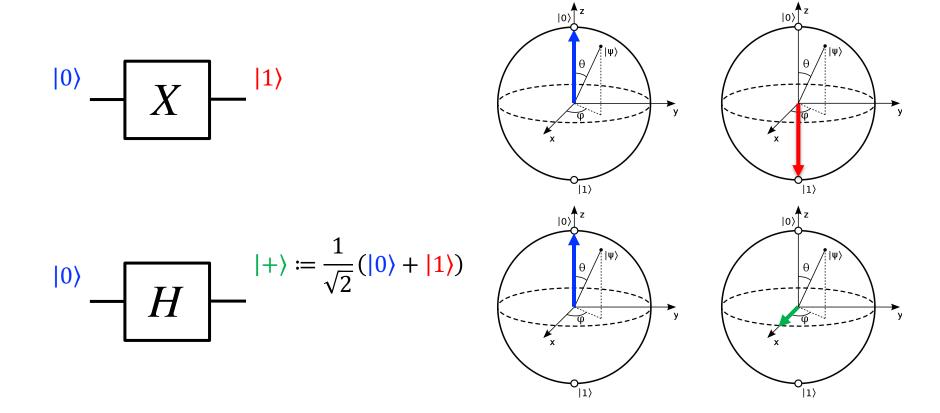


Hadamard

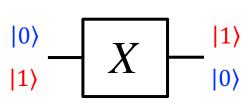


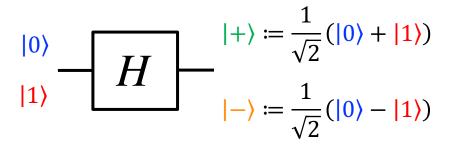
- Unitary operations represented by unitary matrices
- All quantum gates are reversible, e.g. $HH^{\dagger} = I$
- Universal gate set {H,S,T,CNOT}

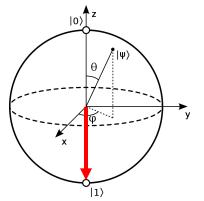
Single-qubit gates

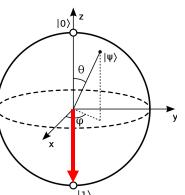


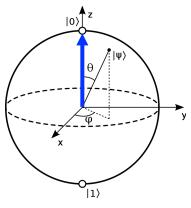
Single-qubit gates

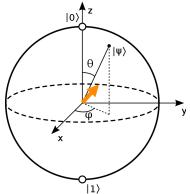




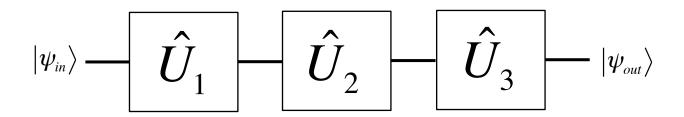








Single-qubit circuits



• Single-qubit gates \widehat{U}_k are **unitary matrices**, i.e.

$$\widehat{U}_k \widehat{U}_k^{\dagger} = \widehat{U}_k^{\dagger} \widehat{U}_k = \widehat{I}$$

Quantum circuits are sequences of matrix-vector multiplications

$$|\psi_{out}\rangle = \widehat{U}_3 \widehat{U}_2 \widehat{U}_1 |\psi_{in}\rangle$$

Multi-qubit states

•
$$|\psi_0\rangle = \alpha_0|0\rangle + \beta_0|1\rangle = \alpha_0 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta_0 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

•
$$|\psi_1\rangle = \alpha_1|0\rangle + \beta_1|1\rangle = \alpha_1\begin{pmatrix}1\\0\end{pmatrix} + \beta_1\begin{pmatrix}0\\1\end{pmatrix}$$

Tensor product

$$|A\rangle \otimes |B\rangle = \begin{bmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{bmatrix}$$

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

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

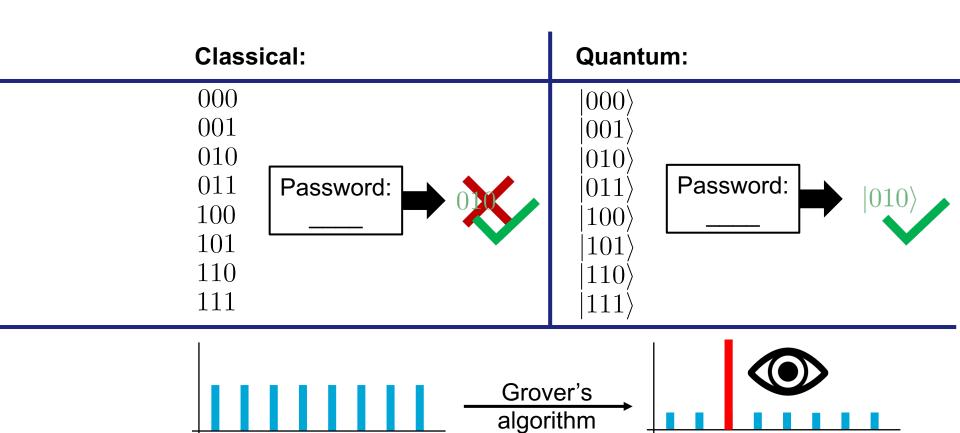
Multi-qubit states, cont'd

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 word 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 measuring
- A single run of a quantum circuit is not very useful; many runs are required to measure the correct answer to the problem with sufficient certainty

Example: 3-bit password



Multi-qubit gates

$$|\Psi_{in}\rangle$$
 $|\Psi_{out}\rangle = H \otimes I |\Psi_{in}\rangle$ $|\Psi_{out}\rangle = H \otimes I |\Psi_{in}\rangle$

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

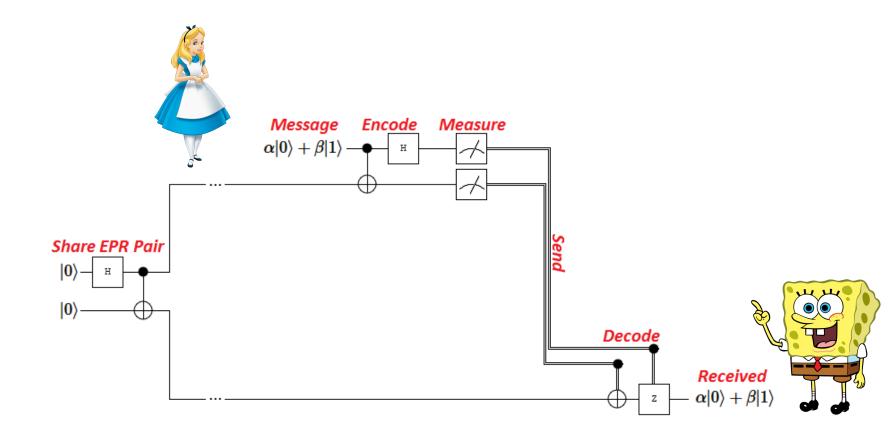
Basic concepts of quantum computing

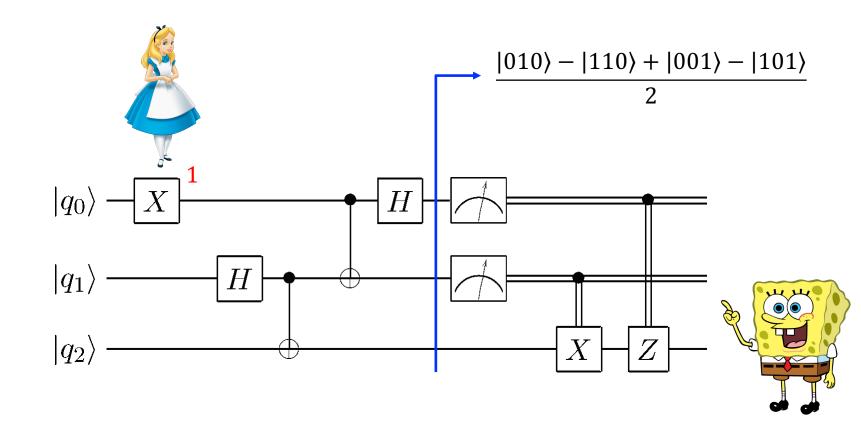
SIMPLE QUANTUM ALGORITHMS

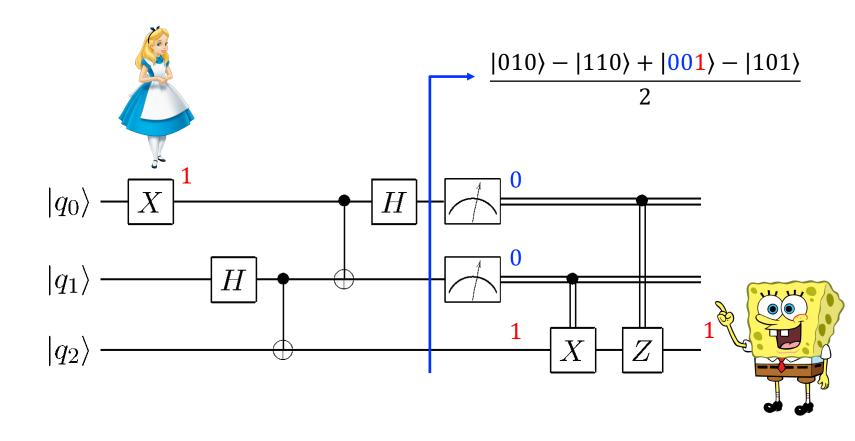
Bell state

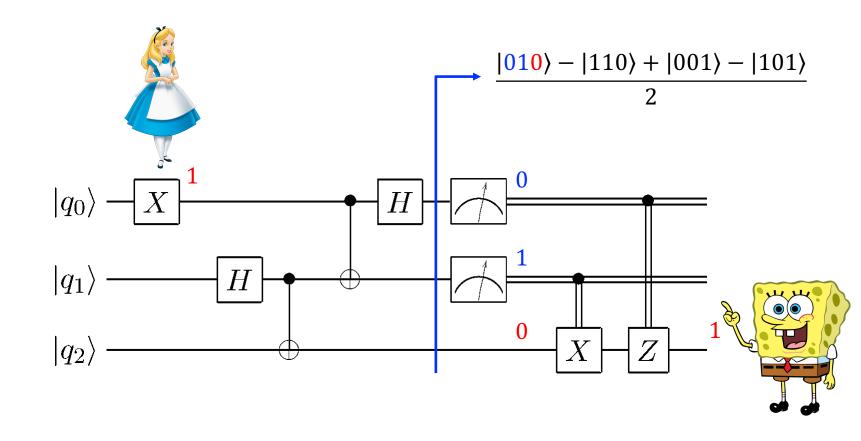
$$CNOT(H \otimes I)|00\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

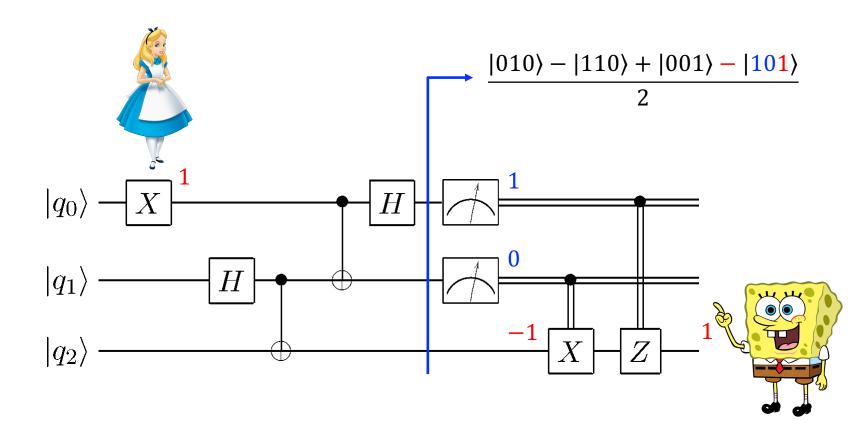
 The Bell state is maximally entangled. By measuring one of the two qubits one knows the value of the other qubit without a further measurement

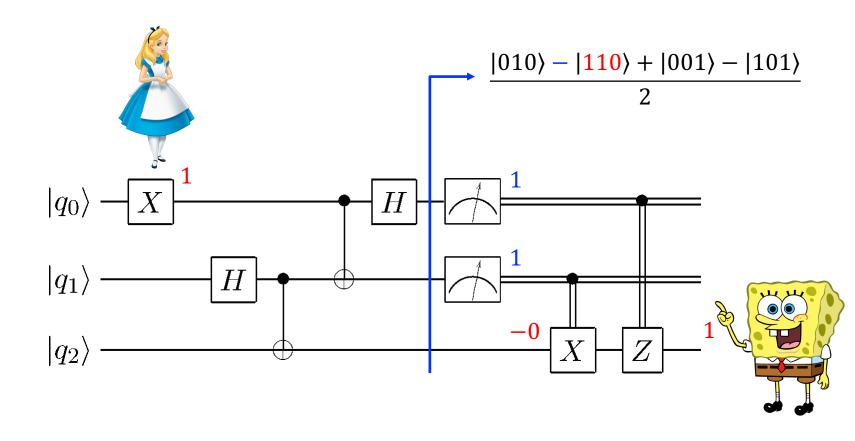




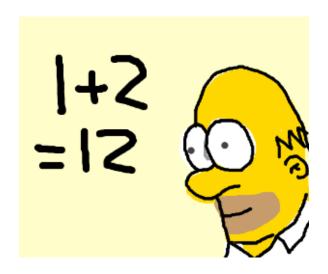




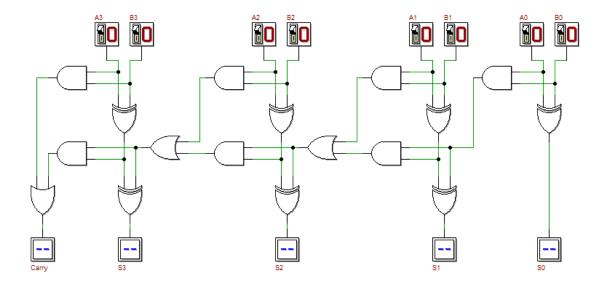




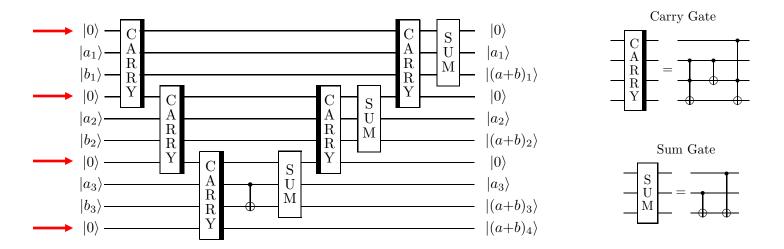
How difficult can it be to add two integers?



Classical integer adder

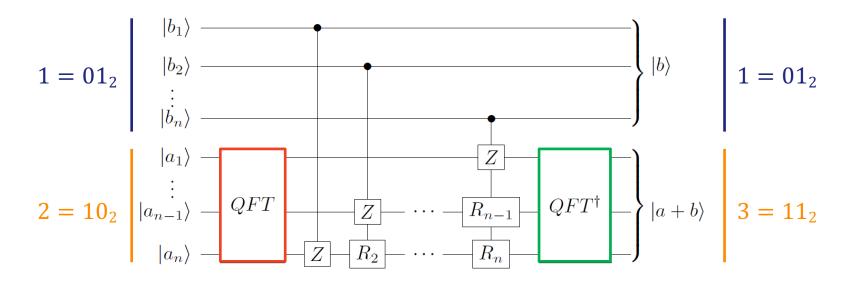


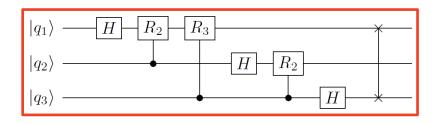
A first quantum integer adder

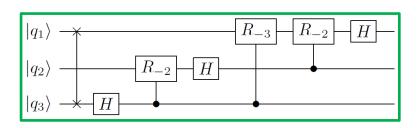


n extra ancilla qubits needed ⊗

Another quantum integer adder







Towards a practical quantum integer adder

1000 QX simulator runs with depolarizing noise error model

•	0,1		$10^{-\frac{3}{2}}$		0,01		$10^{-\frac{5}{2}}$		
QInt <n></n>	1 2 3 4 5 6	0.27045 0.134061 0.0601436 0.0336509	0.3793 0.221523 0.112097 0.0611537	0.50545 0.165182 0.0683512 0.0351125	0.2752 0.209176 0.116162 0.0589036	0.78965 0.451353 0.191802 0.064375 0.0224336 0.00798384	0.1233 0.134284 0.105916 0.0645881 0.031892 0.0176539	0.92285 0.762621 0.540766 0.306778 0.154869 0.0654961	0.0463 0.0570876 0.0754021 0.0802711 0.0575671 0.033179
	8					$\begin{array}{c} 0.00398747 \\ 0.00254026 \end{array}$	0.0076473 0.00363275	0.0252142 0.00834128	$\begin{array}{c} 0.0167067 \\ 0.00823629 \end{array}$

Standard circuit: prob. correct (left), largest prob. wrong answer (right)

Towards a practical quantum integer adder

1000 QX simulator runs with depolarizing noise error model

•	0,1		$10^{-\frac{3}{2}}$		0,01		$10^{-\frac{5}{2}}$		
QInt <n></n>	1 2 3 4 5 6	0.29475 0.110416 0.0581316 0.0259028	0.3695 0.230068 0.114572 0.0583002	0.54555 0.239152 0.096711 0.0382769	0.27185 0.203304 0.122477 0.0672328	0.8158 0.569495 0.341537 0.183066 0.0839273 0.0412412	0.11735 0.115691 0.102147 0.0726129 0.0450361 0.0270095	0.93645 0.837026 0.697436 0.543162 0.407117 0.283642	0.04195 0.0445888 0.0509187 0.0579935 0.0574072 0.049151
Ī	7 8					0.0177059 0.00647699	$\begin{array}{c} 0.0131818 \\ 0.00675828 \end{array}$	0.191996 0.116269	$0.0404665 \\ 0.0290022$

Optimized circuit: prob. correct (left), largest prob. wrong answer (right)

Quantum-accelerated scientific computing

NISQ DEVICES, PROGRAMMING MODELS, AND ALGORITHMS

NISQ era

 Noisy Intermediate-Scale Quantum technology arXiv:1801.00862, 2018



John Preskill

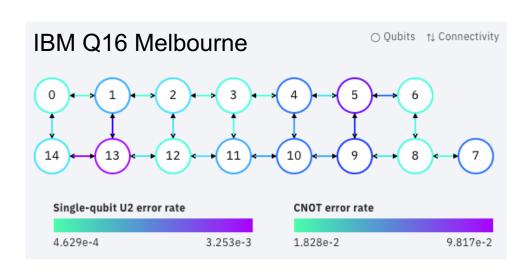
- Noisy emphasizes that we'll have imperfect control over qubits
 - application of $R_{\phi} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$ is inaccurate, i.e. $R_{\phi \pm \epsilon}$
 - quantum state decoheres, i.e. $|\alpha|^2 + |\beta|^2 \neq 1$
- Intermediate-Scale refers to the size of the current and near-future quantum computers which will have between 50 to a few hundred qubits

Quantum processors

Manufacturer	#qubits
IBM	5-53
Rigetti	8-32
Intel	17-49
Google	20-72

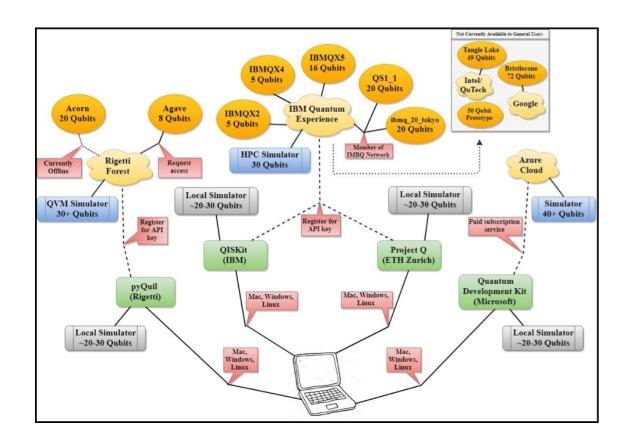
In-memory computing

 Optimal placement and routing of information is crucial; many extra ops

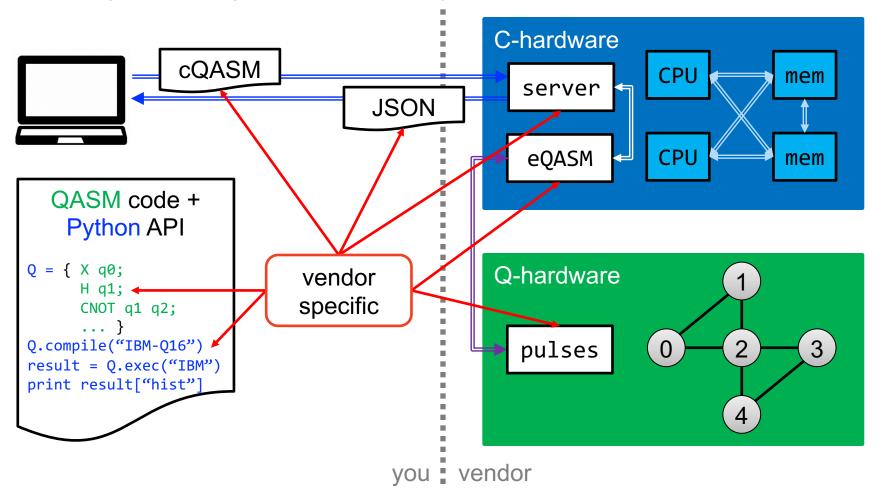


Rigetti's Aspen-7-28Q-A

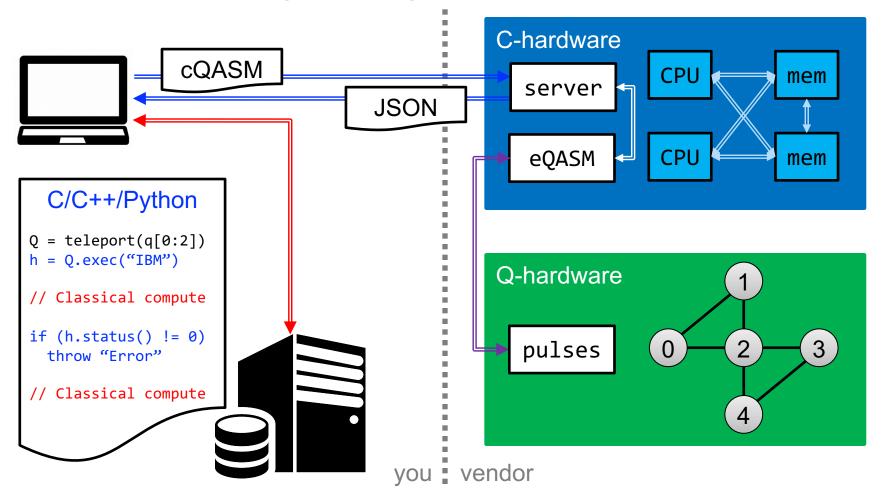
Quantum software platforms



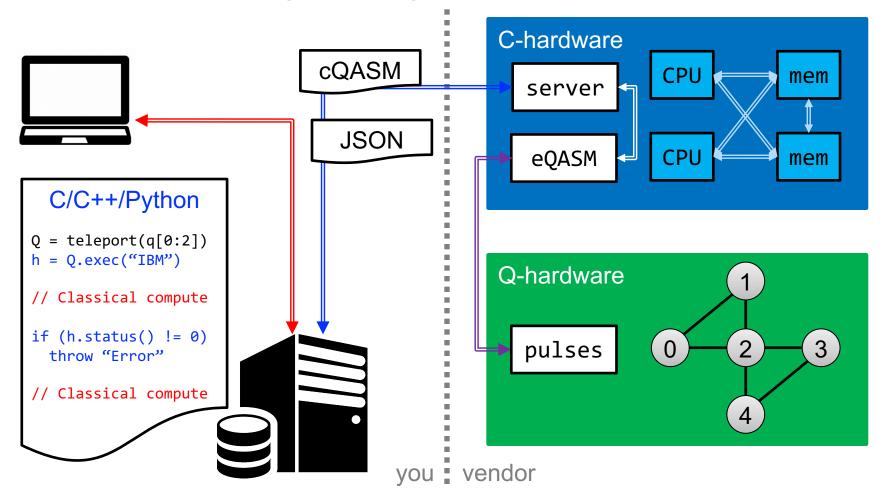
Q-programming model – today



Q-accelerated programming model – our vision



Q-accelerated programming model – our vision



Quantum algorithms with potential use in SciComp

Quantum linear solvers

- HHL-type 'solver' algorithms: $x^{\dagger}Mx$ such that Ax = b
 - sparse matrices [Harrow, Hassidim, Lloyd 2009] $O(\log(N)\kappa^2/\epsilon)$
 - dense matrices [Wossnig et al. 2018] $O(\sqrt{N}\log(N)\kappa^2/\epsilon)$
- Hybrid Variational QC Algorithms (HVQCA)
 - sparse matrices [Bravo-Prieto et al. 2019 & Xu et al. 2019] linear scaling in κ and super-linear scaling in #qubits

Quantum algorithms with potential use in SciComp, cont'd

Quantum algorithms for ...

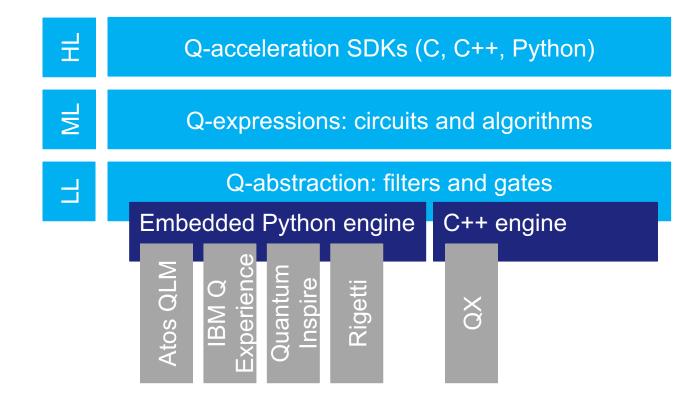
- linear differential equations [Berry 2010, Xin et al. 2018]
- nonlinear differential equations [Leyton, Osborne 2008]
- Poisson equation [Cao et al. 2013]
- principal component analysis [Lloyd et al. 2014]
- data fitting [Wiebe et al. 2012]
- machine learning [Lloyd et al. 2013, Adcock et al. 2015,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

LibKet: The Kwantum expression template LIBrary

DESIGN PRINCIPLES

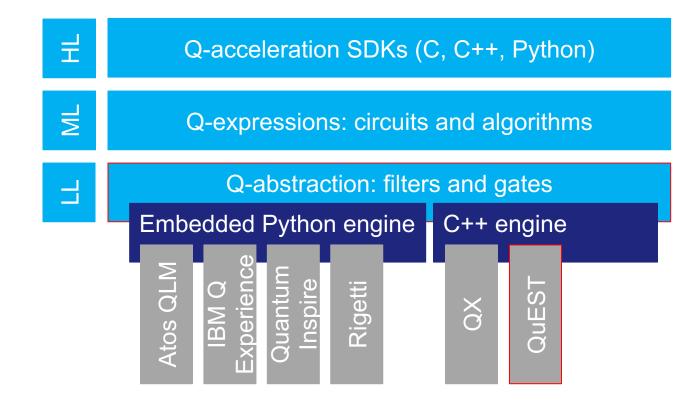


Kwantum expression template LIBrary





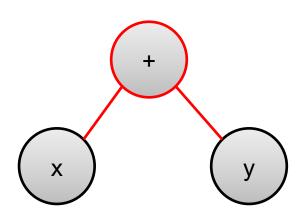
Kwantum expression template LIBrary



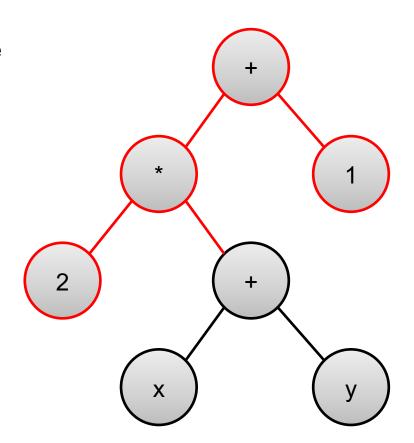
```
Vector x(n), y(n);
```



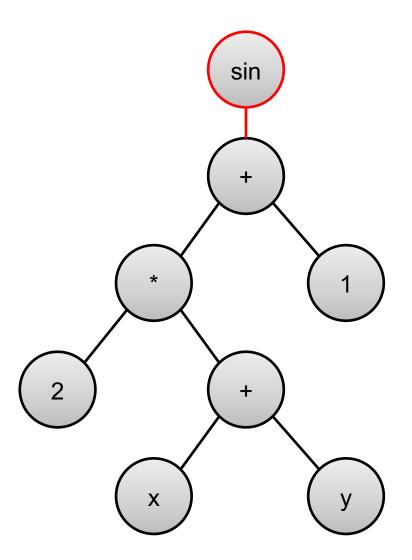
```
Vector x(n), y(n);
auto e0 = x + y;
```



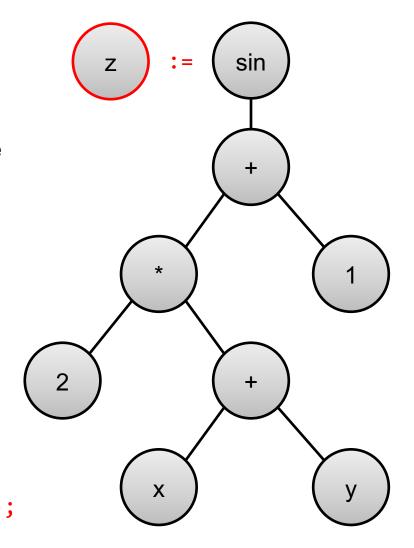
```
Vector x(n), y(n);
auto e0 = x + y;
auto e1 = 2*e0 + 1;
```



```
Vector x(n), y(n);
auto e0 = x + y;
auto e1 = 2*e0 + 1;
auto e2 = sin(e1);
```



```
Vector x(n), y(n);
auto e0 = x + y;
auto e1 = 2*e0 + 1;
auto e2 = sin(e1);
Vector z = e2;
-> z[i] = sin(2*(x[i]+y[i])+1);
```



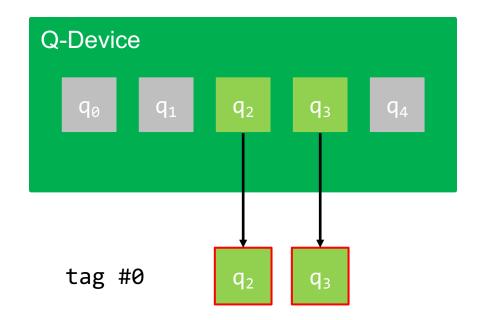
```
auto f0 = select<0,2,3>();
```



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

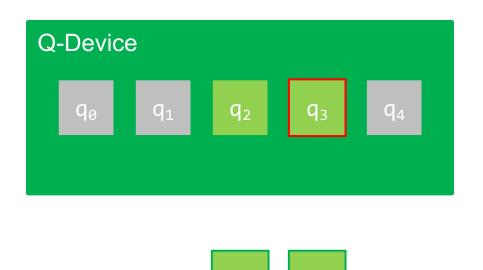


```
auto f0 = select<0,2,3>();
auto f1 = range<1,2>(f0);
auto f2 = tag<0>(f1);
```



 Starting from the full Q-memory filters restrict qubits step by step

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

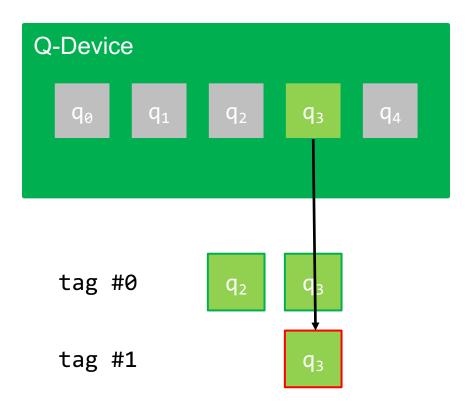


 q_2

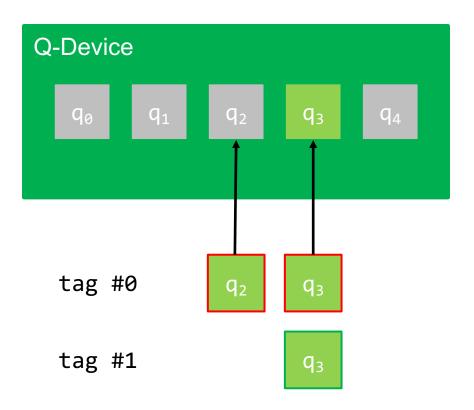
 q_3

tag #0

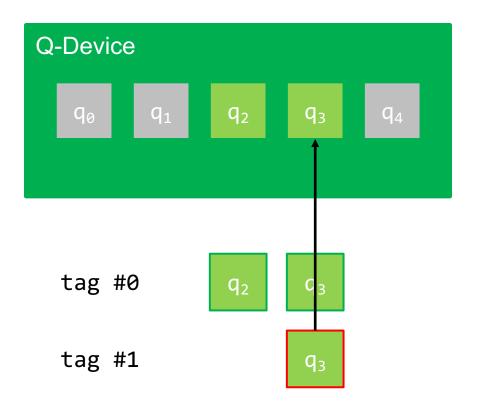
```
auto f0 = select<0,2,3>();
auto f1 = range<1,2>(f0);
auto f2 = tag<0>(f1);
auto f3 = qubit<1>(f2);
auto f4 = tag<1>(f3);
```



```
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);
```



 Gates apply to all qubits of the current filter chain (SIMD-ish)

```
q<sub>0</sub>
```



 q_2

 q_3

 q_4

 Gates apply to all qubits of the current filter chain (SIMD-ish)

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

q₀

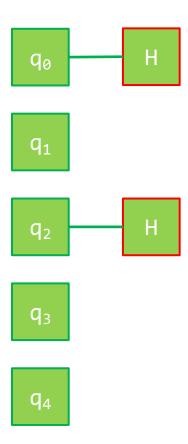
 q_1

 q_2

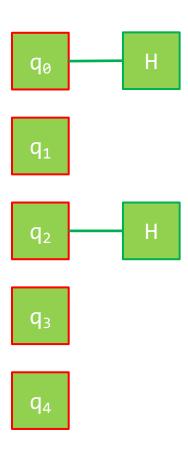
 q_3

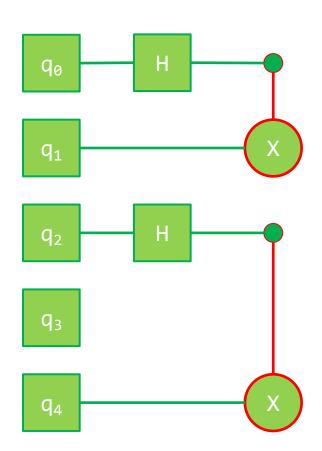
 q_4

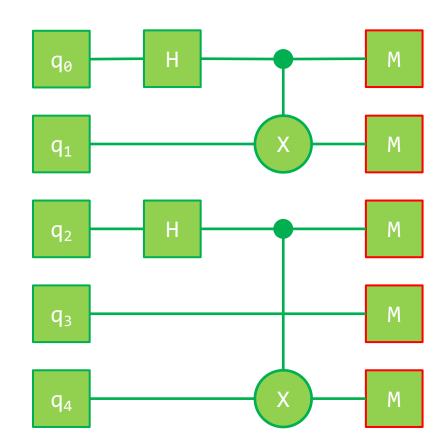
```
auto e0 = init();
auto e1 = sel<0,2>(e0);
auto e2 = h(e1);
```



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

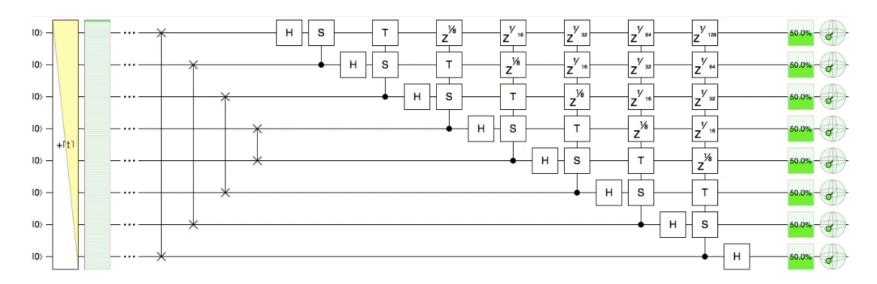






Circuits – pre-cooked quantum building blocks

Generic quantum algorithms that can be applied to registers of arbitrary size



Rule-based optimization

Unitarity of quantum gates

$$S \circ S^{\dagger} = S^{\dagger} \circ S = id$$

auto expr = s(sdag(...));

Template metaprogramming

```
template<class Expr>
auto s(Expr&& expr)
{
    return QGate_S(expr);
}
```

Rule-based optimization

Unitarity of quantum gates

$$S \circ S^{\dagger} = S^{\dagger} \circ S = id$$

Template metaprogramming

```
template<class Expr>
auto s(Expr&& expr)
{
    return QGate_S(expr);
}
```

```
auto expr = ...;
```

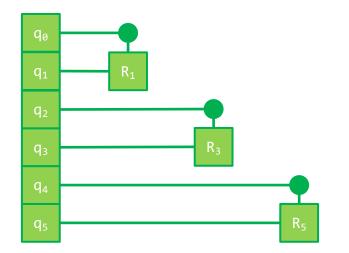
Explicit template specialization

```
template<>
  auto s(QGate_Sdag&& expr)
  {
  return expr.getSubexpr();
}
```

Compile-time loops

For-loop call

```
auto expr =
static_for<1,5,2,body>(...);
```



For-loop body

```
struct body
  template<size_t k,</pre>
           class Expr>
  static constexpr auto
  func(Expr&& expr) noexcept
    return crk<k>(
      sel<k-1>(all( )),
      sel<k >(all(expr)));
```

Advanced techniques

- Hook gate for user-defined mini-circuits
- Just-in-time compilation of run-time generated quantum expressions

Work in progress

- Decomposition gates, e.g. $U = R_z(\varphi_1)R_y(\varphi_2)R_z(\varphi_3)$
- QInteger and QPosit arithmetics
- C and Python API using JIT compilation

FPGA-ish 'synthesis'

Generic quantum expression

```
auto expr = qft(init());
is independent of
```

- Q-device type
- Q-memory size (#qubits)
- concrete input data

FPGA-ish 'synthesis'

- Generic quantum expression auto expr = qft(init()); is independent of
 - Q-device type
 - Q-memory size (#qubits)
 - concrete input data
- Q-device specific kernel code
 QData<6, cQASMv1> data;
 cout << expr(data);

```
version 1.0
qubits 6
h q[0]
cr q[1], q[0], 1.570796326794896558
cr q[2], q[0], 0.785398163397448279
cr q[3], q[0], 0.392699081698724139
cr q[4], q[0], 0.196349540849362070
cr q[5], q[0], 0.098174770424681035
h q[1]
cr q[2], q[1], 1.570796326794896558
cr q[3], q[1], 0.785398163397448279
cr q[4], q[1], 0.392699081698724139
cr q[5], q[1], 0.196349540849362070
h q[2]
cr q[3], q[2], 1.570796326794896558
cr q[4], q[2], 0.785398163397448279
cr q[5], q[2], 0.392699081698724139
h q[3]
cr q[4], q[3], 1.570796326794896558
cr q[5], q[3], 0.785398163397448279
h q[4]
cr q[5], q[4], 1.570796326794896558
h q[5]
swap q[0], q[5]
swap q[1], q[4]
swap q[2], q[3]
```

Quantum-Inspire

FPGA-ish 'synthesis'

- Generic quantum expression auto expr = qft(init());is independent of
 - Q-device type
 - Q-memory size (#qubits)
 - concrete input data
- Q-device specific kernel code QData<6, openQASMv2> data; cout << expr(data);</p>

```
version 1.0
qubits 6
h q[0]
cr q[1], q[0], 1.570796326794896558
cr q[2], q[0], 0.785398163397448279
cr q[3], q[0], 0.392699081698724139
cr q[4], q[0], 0.196349540849362070
cr q[5], q[0], 0.098174770424681035
h q[1]
cr q[2], q[1], 1.570796326794896558
cr q[3], q[1], 0.785398163397448279
cr q[4], q[1], 0.392699081698724139
cr q[5], q[1], 0.196349540849362070
h q[2]
cr q[3], q[2], 1.570796326794896558
cr q[4], q[2], 0.785398163397448279
cr q[5], q[2], 0.392699081698724139
h q[3]
cr q[4], q[3], 1.570796326794896558
cr q[5], q[3], 0.785398163397448279
h q[4]
cr q[5], q[4], 1.570796326794896558
h q[5]
swap q[0], q[5]
swap q[1], q[4]
swap q[2], q[3]
```

```
OPENQASM 2.0;
include "qelib1.inc";
qreg q[6];
creg c[6];
h q[0];
cu1(1.570796326794896558) q[1], q[0];
cu1(0.785398163397448279) q[2], q[0];
cu1(0.392699081698724139) q[3], q[0];
cu1(0.196349540849362070) q[4], q[0];
cu1(0.098174770424681035) q[5], q[0];
h q[1];
cu1(1.570796326794896558) q[2], q[1];
cu1(0.785398163397448279) q[3], q[1];
cu1(0.392699081698724139) q[4], q[1];
cu1(0.196349540849362070) q[5], q[1];
cu1(1.570796326794896558) q[3], q[2];
cu1(0.785398163397448279) q[4], q[2];
cu1(0.392699081698724139) q[5], q[2];
h q[3];
cu1(1.570796326794896558) q[4], q[3];
cu1(0.785398163397448279) q[5], q[3];
h q[4];
cu1(1.570796326794896558) q[5], q[4];
h q[5];
swap q[0], q[5];
swap q[1], q[4];
swap q[2], q[3];
```

CUDA-ish stream execution model

- High latency is caused by
 - Python-based vendor tools and complexity of the process
 - remote access to cloud-based
 Q-devices with waiting queues

```
// Blocking execution
QJob* job = data.execute(...);
// Result as JSON object
json result = job->get();
```

CUDA-ish stream execution model

- High latency is caused by
 - Python-based vendor tools and complexity of the process
 - remote access to cloud-based
 Q-devices with waiting queues
- Asynchronous execution
 - hides latencies by continuing the classical program flow

```
// Non-blocking execution
QJob* job = data.execute_async(...);
// do other tasks
// Wait for completion
job->wait();
```

CUDA-ish stream execution model

- High latency is caused by
 - Python-based vendor tools and complexity of the process
 - remote access to cloud-based
 Q-devices with waiting queues
- Asynchronous execution
 - hides latencies by continuing the classical program flow
 - enables concurrent execution of kernels via multiple streams

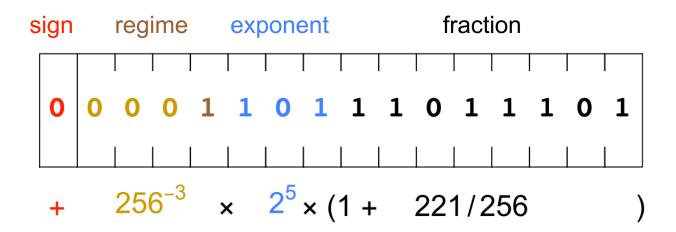
```
QStream stream0, stream1;
QJob* job0 =
  data0.execute_async(stream0,...);
QJob* job1 =
  data1.execute async(stream1,...);
// do other tasks
if (job0->query()) { ... }
if (job1->query()) { ... }
```

LibKet: The Kwantum expression template LIBrary

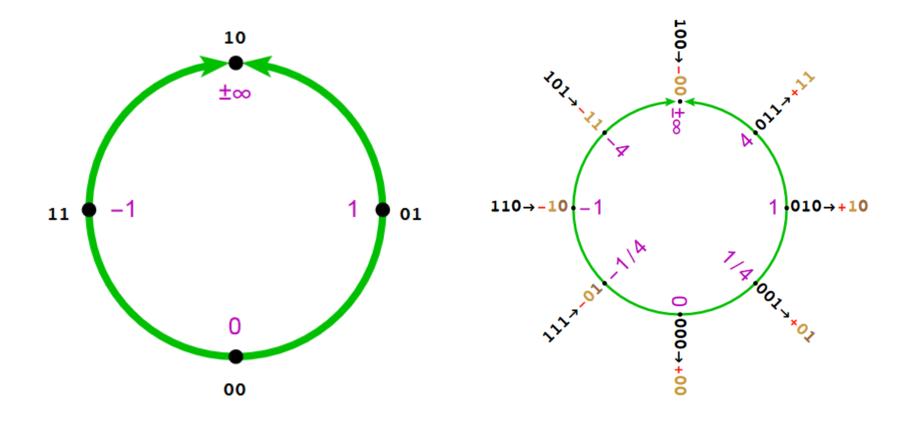
ONGOING DEVELOPMENTS

Real-valued data

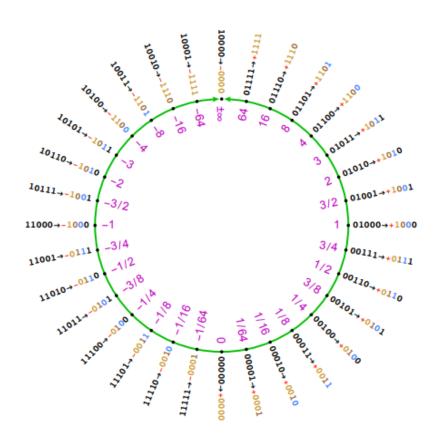
- IEEE-754 floating points require 32-64 qubits per datum → impractical
- Encoding real-number in a single qubit → tempting but not succeeded yet
- More (qu)bit efficient number formats → Posits (Type III UNUMs)



Posits



Posit arithmetic



Example:

$$3 = +1011$$

 $4 = +1100$

$$8 = +1101$$

3

Initialization

3

4

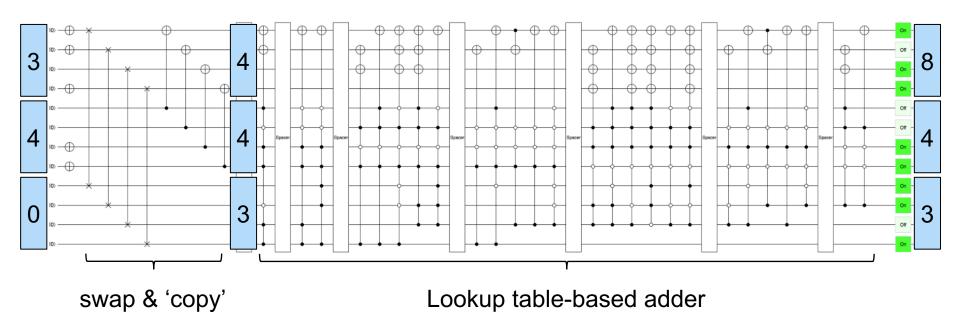
ook-up table based adder

4

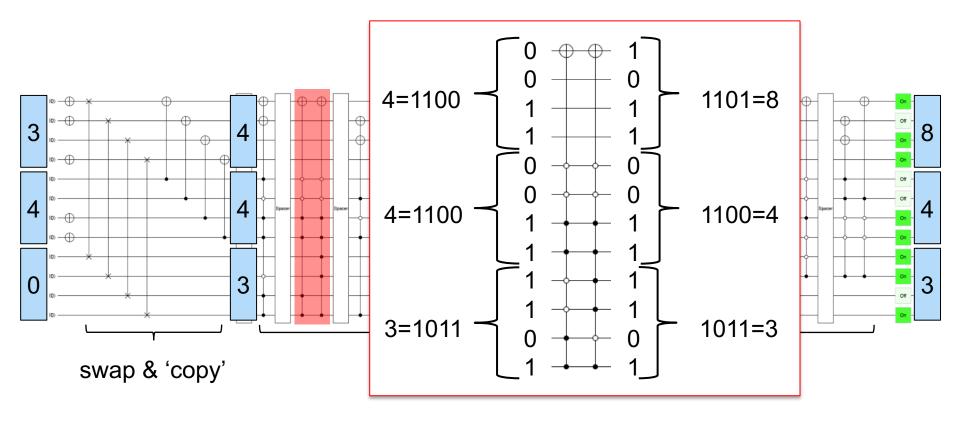
8

3

Posit arithmetic on quantum computers



Posit arithmetic on quantum computers



Conclusion



A cross-platform SDK for Q-accelerated scientific computing

- Rapid prototyping and testing of quantum expressions
- Seamless integration into (C-accelerated) applications

Ongoing work

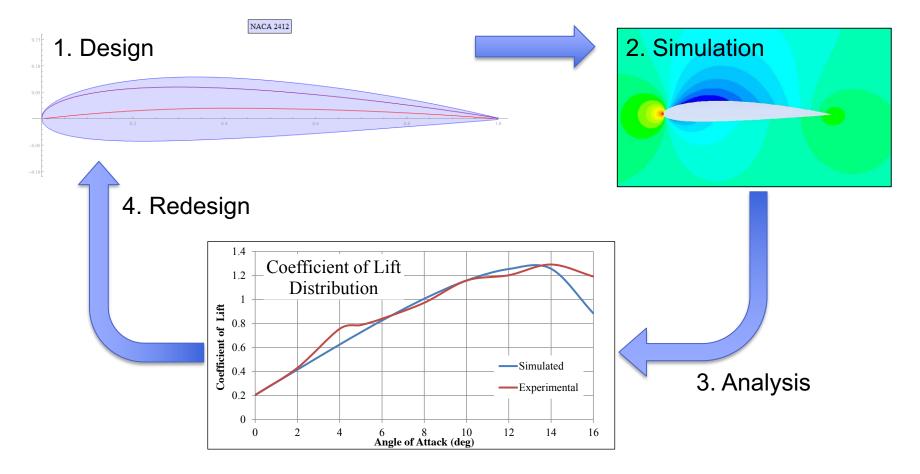
- Implementation of HHL and QInteger/QPosit arithmetics
- Cloud platform https://INGInious.ewi.tudelft.nl

Publications

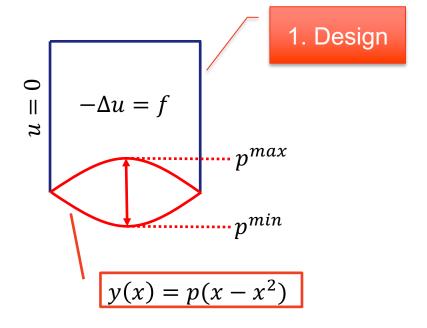
- MM, Schalkers: A cross-platform programming framework for quantumaccelerated scientific computing. Submitted to ICCS 2020
- Driebergen, MM: A novel quantum algorithm for adding real-valued numbers using posit arithmetic. Submitted to RC 2020

Extra Slides

Simulation-based design and analysis cycle



Academic model problem



4. Redesign

Problem: Minimize the difference

$$d_h = u_h - u_h^*$$

between the solution u_h and a given profile u_h^* w.r.t. 3. Analysis

$$\mathcal{C}(d_h, p) = d_h^T M d_h$$

such that d_h solves 2. Simulation

$$A_h d_h = f_h - A_h u_h^*$$