# Quantum-accelerated scientific computing finally made easy

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#### 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

# **QUANTUM BITS AND GATES**

Basic concepts of quantum computing

### 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)

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

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|<sup>2</sup> and |β|<sup>2</sup> are the probabilities of measuring the basis states |0⟩ and |1⟩, respectively

#### Single-qubit states

Bloch sphere

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

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



#### **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



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

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

### Single-qubit gates



### Single-qubit gates



#### Single-qubit circuits

$$|\psi_{\scriptscriptstyle in}
angle - \hat{m{U}}_1 - \hat{m{U}}_2 - \hat{m{U}}_3 - |\psi_{\scriptscriptstyle out}
angle$$

• Single-qubit gates  $\hat{U}_k$  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

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

$$\begin{aligned} |\alpha_0 \alpha_1|^2 + |\alpha_0 \beta_1|^2 + |\beta_0 \alpha_1|^2 + |\beta_0 \beta_1|^2 = \\ |\alpha_0|^2 (|\alpha_1|^2 + |\beta_1|^2) + |\alpha_1|^2 (|\alpha_1|^2 + |\beta_1|^2) = 1 \end{aligned}$$

#### 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  $\gamma$ '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



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

## SIMPLE QUANTUM ALGORITHMS

Basic concepts of quantum computing

#### 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



D.E. Searls, Computer Organization & Systems, dsearls.org

A first quantum integer adder



n extra ancilla qubits needed 😕

Cuccaro et al.: A new quantum ripple-carry addition circuit, arXiv:quant-ph/0410184, 2004

#### Another quantum integer adder







Draper: Addition on a quantum computer, arXiv:quant-ph/0008033, 2000

#### Towards a practical quantum integer adder

#### 1000 QX simulator runs with depolarizing noise error model

-	0,1		$10^{-\frac{3}{2}}$		0,01		$10^{-\frac{5}{2}}$		
-	1	0.27045	0.3793	0.50545	0.2752	0.78965	0.1233	0.92285	0.0463
^	2	0.134061	0.221523	0.165182	0.209176	0.451353	0.134284	0.762621	0.0570876
	3	0.0601436	0.112097	0.0683512	0.116162	0.191802	0.105916	0.540766	0.0754021
Ť	4	0.0336509	0.0611537	0.0351125	0.0589036	0.064375	0.0645881	0.306778	0.0802711
Ē	5					0.0224336	0.031892	0.154869	0.0575671
<b>D</b>	6					0.00798384	0.0176539	0.0654961	0.033179
-	7					0.00398747	0.0076473	0.0252142	0.0167067
	8					0.00254026	0.00363275	0.00834128	0.00823629

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

M. Looman: Implementation and Analysis of an Algorithm on Positive Integer Addition for Quantum Computing, Bachelor thesis, 2018

#### Towards a practical quantum integer adder

#### 1000 QX simulator runs with depolarizing noise error model

		$0,\!1$		$10^{-\frac{3}{2}}$		0,01		$10^{-\frac{5}{2}}$	
	1	0.29475	0.3695	0.54555	0.27185	0.8158	0.11735	0.93645	0.04195
$\mathbf{\wedge}$	2	0.110416	0.230068	0.239152	0.203304	0.569495	0.115691	0.837026	0.0445888
C	3	0.0581316	0.114572	0.096711	0.122477	0.341537	0.102147	0.697436	0.0509187
Ť	4	0.0259028	0.0583002	0.0382769	0.0672328	0.183066	0.0726129	0.543162	0.0579935
Ē	5					0.0839273	0.0450361	0.407117	0.0574072
D I	6					0.0412412	0.0270095	0.283642	0.049151
Ŭ	7					0.0177059	0.0131818	0.191996	0.0404665
	8					0.00647699	0.00675828	0.116269	0.0290022

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

M. Looman: Implementation and Analysis of an Algorithm on Positive Integer Addition for Quantum Computing, Bachelor thesis, 2018

## NISQ DEVICES, PROGRAMMING MODELS, AND ALGORITHMS

Quantum-accelerated scientific computing

#### 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



LaRose: Overview and Comparison of Gate Level Quantum Software Platforms, arXiv:1807.02500, 2018

#### 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, …]

# **DESIGN PRINCIPLES**

LibKet: The Kwantum expression template LIBrary



# Kwantum expression template LIBrary



MM, Schalkers: LibKet: A cross-platform programming framework for quantum-accelerated scientific computing, submitted to ICCS 2020



# Kwantum expression template LIBrary



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 C++ metaprogramming technique to create lightweight expressions whose evaluation is delayed until their values are really needed

Vector x(n), y(n);



 C++ metaprogramming technique to create lightweight expressions whose evaluation is delayed until their values are really needed

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



 C++ metaprogramming technique to create lightweight expressions whose evaluation is delayed until their values are really needed

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



 C++ metaprogramming technique to create lightweight expressions whose evaluation is delayed until their values are really needed

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



 C++ metaprogramming technique to create lightweight expressions whose evaluation is delayed until their values are really needed

```
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);



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

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



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

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



 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);



 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);
```



```
tag #0
```



 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);
auto f4 = tag<1>(f3);
```



 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); auto f4 = tag<1>(f3); auto f5 = gototag<0>(f4);



 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);
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)

auto e0 = init();



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

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);
```







#### Circuits – pre-cooked quantum building blocks

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

auto expr = qft(...);



#### **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

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- Generic quantum expression auto expr = qft(init());
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    - concrete input data
- Q-device specific kernel code
   QData<6, cQASMv1> data;
   cout << expr(data);</li>

```
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);</li>

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]; h q[2]; 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];

Quantum-Inspire

**IBM Q Experience** 

#### 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()) { ... }
```

# **ONGOING DEVELOPMENTS**

LibKet: The Kwantum expression template LIBrary
### Real-valued data

- IEEE-754 floating points require 32-64 qubits per datum  $\rightarrow$  impractical
- Encoding real-number in a single qubit  $\rightarrow$  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



## Posit arithmetic on quantum computers



T. Driebergen: Designing a Quantum Algorithm for Real-Valued Addition Using Posit Arithmetic, BSc Thesis, TU Delft, 2019

# Posit arithmetic on quantum computers



T. Driebergen: Designing a Quantum Algorithm for Real-Valued Addition Using Posit Arithmetic, BSc Thesis, TU Delft, 2019

## 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 <u>https://INGInious.ewi.tudelft.nl</u>

#### 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



Matsson et al. Aerodynamic Performance of the NACA 2412 Airfoil at Low Reynolds Number, 2016 ASEE Annual Conference & Exposition

## 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  $C(d_h, p) = d_h^T M d_h$ 

such that  $d_h$  solves 2. Simulation  $A_h d_h = f_h - A_h u_h^*$