Quantum-accelerated scientific computing

Matthias Möller

Delft Institute of Applied Mathematics

About me

- Assistant Professor in Numerical Analysis at TU Delft since 2013 (before TU Dortmund)

- Research interests:
  - FEM/IGA for (compressible) flow problems
  - High-resolution and high-order methods
  - Efficient multilevel solution methods
  - Hybrid particle mesh methods (MPM, OTM)
  - Heterogeneous high-performance computing
  - Quantum-accelerated scientific computing

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State-of-the art in quantum-accelerated scientific computing and how we try to advance it

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Accelerated computing

- Heterogeneous compute nodes with multi-socket, multi-core CPUs and general-purpose accelerators (GPUs, FPGAs, vector processors, …)
- **Current and future trend**: special-purpose accelerators (Google's TPUs, ASICs, …)
- **Vision**: use QPUs as functional accelerators
- **Philosophy**: Hardware-oriented Numerics = co-design of hardware-aware numerical methods and their hardware-optimized H^2PC implementation

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QPUs

- **Discrete gate model**:
  - Google “Bristlecone”: 72(?) hw-qubits
  - IBM Q Experience: 4-16/20(?) hw-qubits
  - Intel ”Tangle Lake”: 49(?) hw-qubits
  - Rigetti: 19/128(?) hw-qubits
  - Atos QLM: 40 sw-qubits
  - QuTech QX/OpenQL: 26 sw-qubits
  - TNO Quantum Inspire: 31-37 sw-qubits

20 hw
40 sw
qubits

- ~~**Quantum annealing**:~~
  - ~~D-Wave system 2000Q: 2048/5000(?) qubits~~

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Quantum SDKs

- **Quantum Assembly/Instruction languages**:
  - AQASM: Atos QML
  - cQASM: TNO Quantum Inspire, QuTech QX
  - OpenQASM: IBM Q Experience, Google
  - Quil: Rigetti simulator and cloud platform

- **SDKs** (in Python):
  - pyAqasm: Atos (AQASM in/out)
  - pyQuil: Rigetti (Quil in/out)
  - Circ: Google (OpenQASM out, no in)
  - QX/OpenQL (C++): QuTech (cQASM in/out)
  - ProjectQ: ETHZ (no xQASM in/out)
  - QisKit: IBM (OpenQASM in/output)
  - Quantum Development Kit (Q#): Microsoft (OpenQASM in/out)

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Proprietary workflow

- Python script → [xQASM kernel] → QPU-optimized binary code → QSim/QComputer → post-processing in Python
- **Pros:**
  - Exploitation of knowledge of QPU internals in optimization
  - Flat learning curve to get started with basic quantum algorithm
- **Cons**:
  - Proprietary Q-toolchains (compilers, optimizers) and workflows
  - Re-inventing the wheel in each SDK (only prototype circuits)
  - No direct comparison of algorithms between QPUs possible
  - None of the tools aims at scientific computing at large scale
  - Investment insecurity (NVIDIA CUDA vs. ATI Stream SDK)

LibKet

|LIB⟩

- Kwantum expression template Library
- Header-only C++14 open-source library (soon) available at https://gitlab.com/mmoelle1/LibKet
- **Planning:** 1st official release before this summer with full support for all aforemention Q-backends
- **Long-term vision**: LibKet becomes the Eigen library of the Q-accelerated scientific computing community

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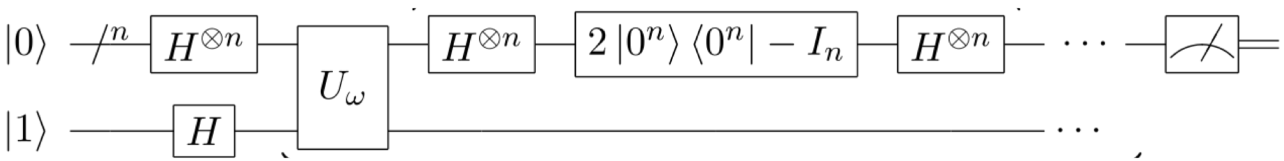
LibKet

|LIB⟩

- Provides C++ wrappers for all basic **quantum gates** and commonly used **circuits** templated over #qubits

```
auto expr = … h(all(x(sel<n>(init()))));
```



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LibKet

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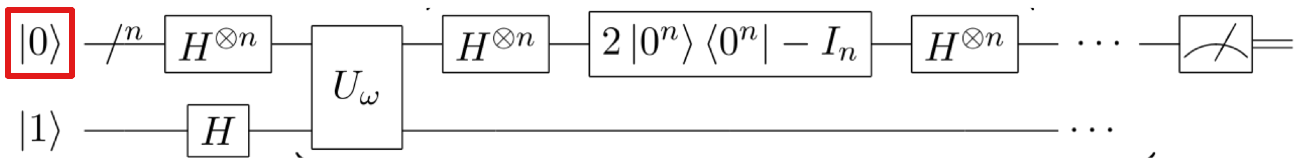

LibKet

$|\text{LIB}\rangle$

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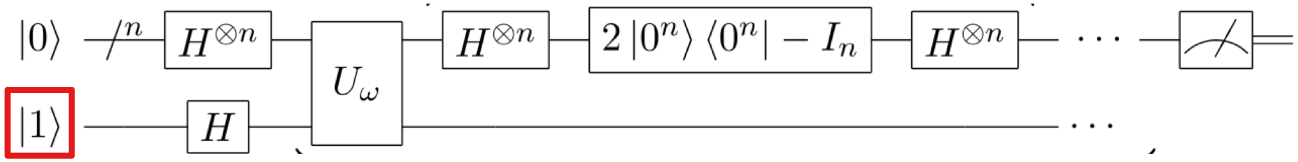

LibKet

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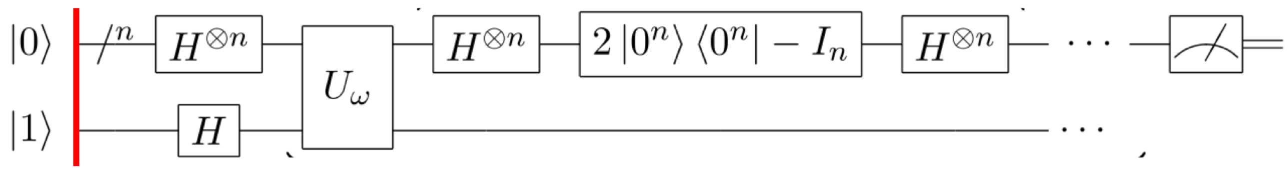

LibKet

|LIB⟩

- Provides wrappers for all basic **quantum gates** and commonly used **circuits** templated over #qubits

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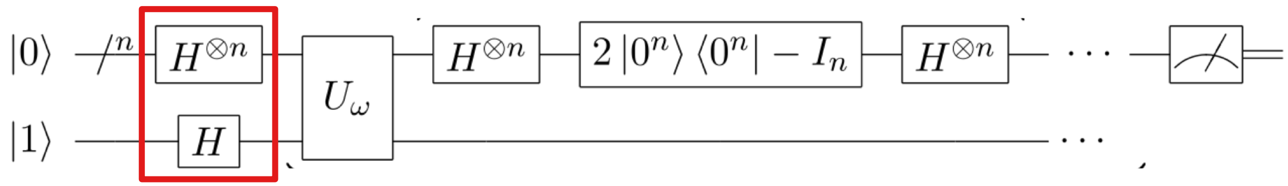

LibKet

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- Synthesizes quantum expressions into **rule-based optimized xQASM (QX/OpenQL) quantum kernels**

```
# cQASM 1.0
version 1.0
qubits 6
x q[5]
h q[0,1,2,3,4,5]
…
```

```
OPENQASM 2.0;
include "qelib1.inc";
qreg q[6];
x q[5];
h q[0];
h q[1];
h q[2];
…
```

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LibKet

|LIB⟩

- Bidirectional communication between C++ host code and Python-based QSim/QComputer environment

```
QData<6, OpenQASMv2> backend;
json result = expr(backend).execute();
cout << result << endl;
```


```
[{"data":{"counts":{"0x0":22,"0x1":15,"0x10":18
,"0x11":11,"0x12":15,"0x13":11,"0x14":14,"0x15"
:20,"0x16":12,"0x17":13,"0x18":15,"0x19":16 ...
```


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LibKet

|LIB⟩

- Will allow end-user to **develop quantum algorithms** from scratch but also to exploit Q-acceleration using ready-to-use **pre-built quantum expressions**

```
auto expr = qft<…>(range<0,5>(init()));
```

- Will provide **intrinsic types and arithmetic ops**:

```
QInt<6>      a(1),   b(1);   a+=b;
QPosit<8,1> a(1.3), b(2.3); a+=b;
```

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LibKet workflow

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- C++ host code
  → auto-generate rule-based optimized xQASM kernel
  → apply proprietary toolchain (compile & execute)
  → import results into C++ host code via JSON objects

- **Pros**:
  - Develop Q-accelerated scientific application in C++ only
  - Develop backend-independent quantum algorithms (QA) just once
  - Exploit all benefits (QPU-optimization) from proprietary toolchains
  - Compare different QPUs at the cost of a single code compilation

- **Cons**: None? Try it yourself and please tell me if any!

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Past and ongoing activities

- **Bachelor projects**:
  - v.d. Lans: Multi-search Groover, Q-add/sub
  - Looman: Q-add with simulated quantum errors QC1.0
  - v.d. Linde: Posit arithmetics

  - Driebergen: Posit arithmetics for QC
  - Ubbes: Quantum Linear Solver Algorithm (QLSA) QC2.0
  - Schalkers (internship at TNO): LibKet, …

- **Collaborations**:
  - TNO, TU Delft Quantum & Computer Eng., SurfSara

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A first quantum algorithm: 1+1=2

- **Integer addition**:
  - a = 1; b = 1; c = a+b; ✗ (no-cloning principle)
  - a = 1; b = 1; a += b; ✓

- **Classical adder circuits**:
  - Must be reversible (all QAs are reversible!)
  - Must be realizable with quantum gates only
  - Should need few ancilla qubits (20-40 qubits)

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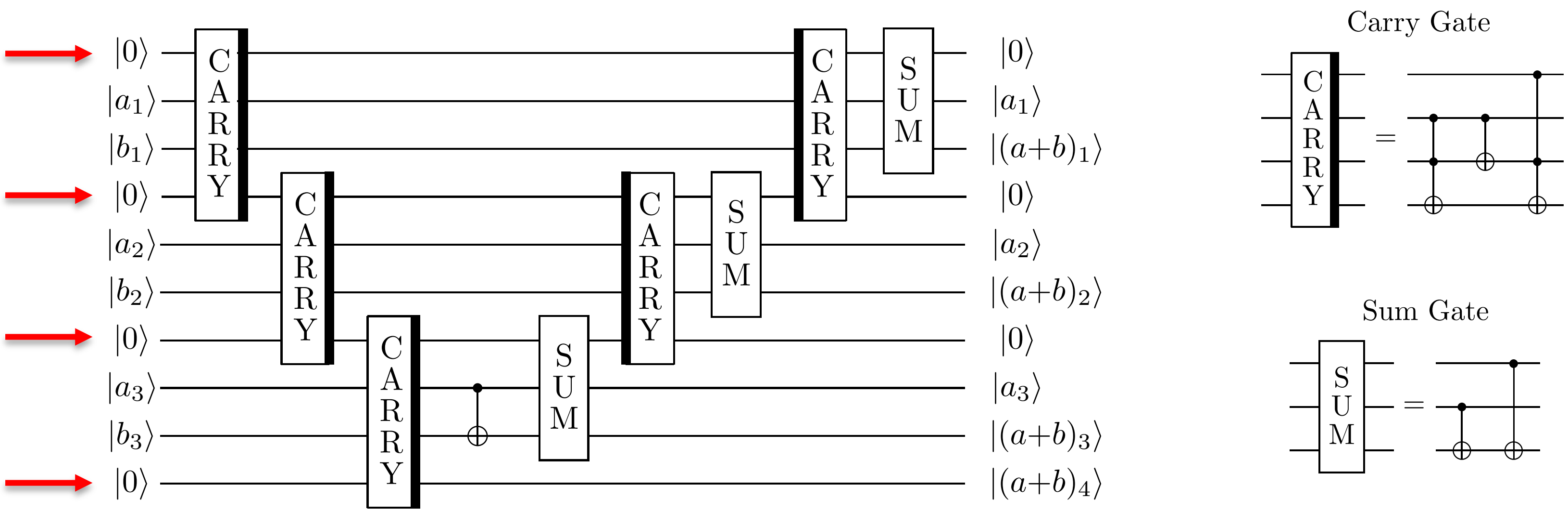
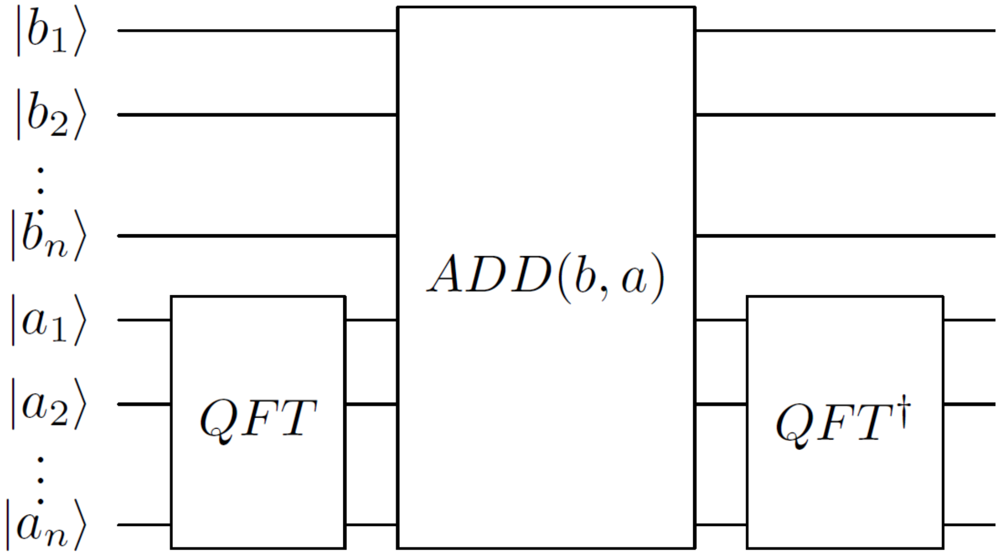
A first quantum algorithm: 1+1=2



n extra ancilla qubits needed ☹

Cuccaro et al.: A new quantum ripple-carry addition circuit (2008)

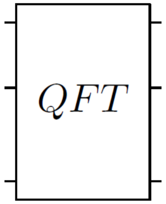
Another quantum algorithm: 1+1=2

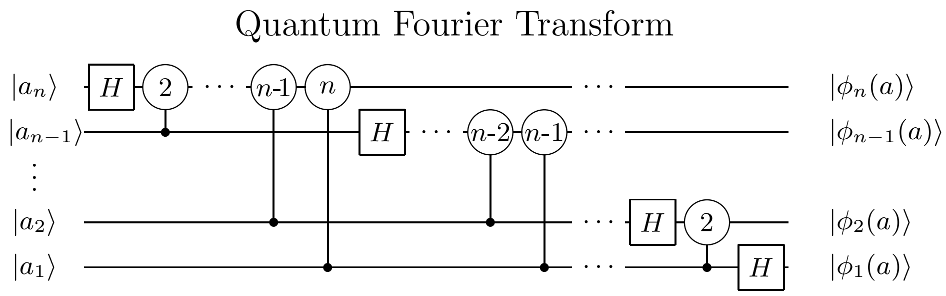


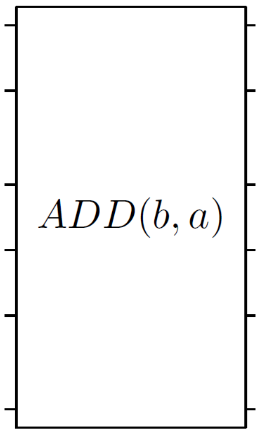
no extra ancilla qubits needed ☺

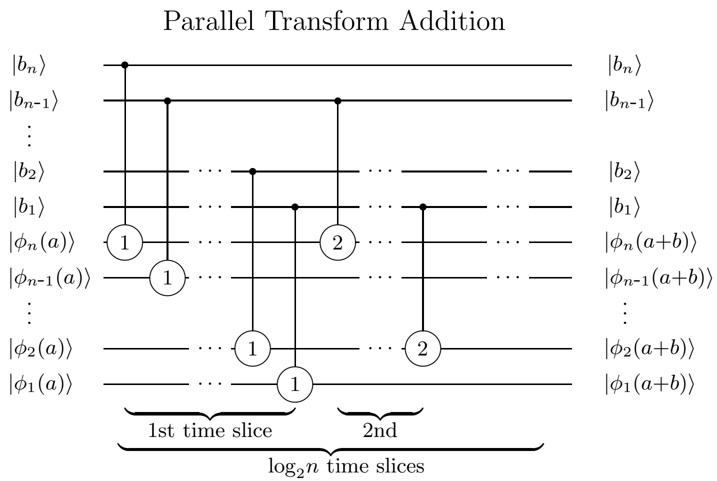
Draper: Addition on a quantum computer (2000)

Another quantum algorithm: 1+1=2









Draper: Addition on a quantum computer (2000)

Using LibKet: 1+1=2

- **LibKet quantum expression**:

```
auto expr =
  qftdag( range<n,n>( add( range<0,n>( all() ),
                           qft( range<n,n>() )
        )           );
```

- Or simply (planned for 1st official release):

```
QInt<6> a(1), b(1); a += b;
```

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Towards practical QC: 1+1 ≅ 2

1000 QX simulator runs with depolarizing noise error model

QInt<n>	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
4	0.0336509	0.0611537	0.0351125	0.0589036	0.064375	0.0645881	0.306778	0.0802711
5					0.0224336	0.031892	0.154869	0.0575671
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)

Looman: Implementation and Analysis of an Algorithm on Positive Integer Addition for Quantum Computing (2018)

Towards practical QC: 1+1 ≅ 2

1000 QX simulator runs with depolarizing noise error model

QInt<n>	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
2	0.110416	0.230068	0.239152	0.203304	0.569495	0.115691	0.837026	0.0445888
3	0.0581316	0.114572	0.096711	0.122477	0.341537	0.102147	0.697436	0.0509187
4	0.0259028	0.0583002	0.0382769	0.0672328	0.183066	0.0726129	0.543162	0.0579935
5					0.0839273	0.0450361	0.407117	0.0574072
6					0.0412412	0.0270095	0.283642	0.049151
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)

Looman: Implementation and Analysis of an Algorithm on Positive Integer Addition for Quantum Computing (2018)

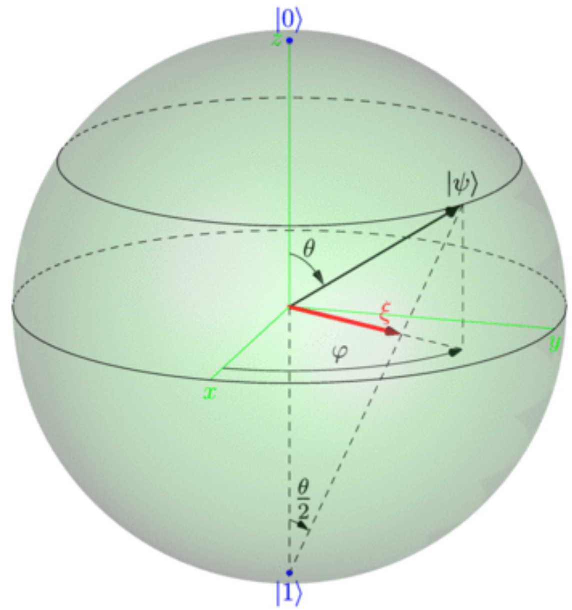
Quantum computing in a nutshell and why it's so difficult to make progress

QC in a nutshell

- **A single qubit state:**

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

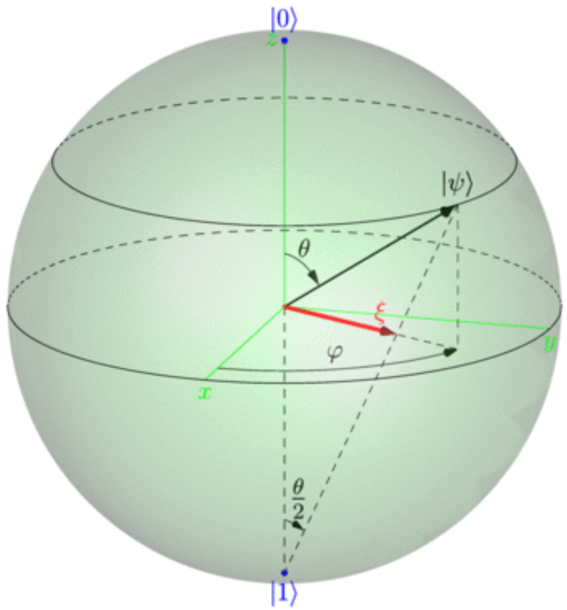
$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$$



QC in a nutshell

- **Hadamard (H) gate:**

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



Unitary operators, i.e. $UU^{\dagger} = I$ or $\langle u, v \rangle_H = \langle Uu, Uv \rangle_H, \forall u, v \in H$

$$H|\psi\rangle = \frac{\alpha + \beta}{\sqrt{2}} |0\rangle + \frac{\alpha - \beta}{\sqrt{2}} |1\rangle$$

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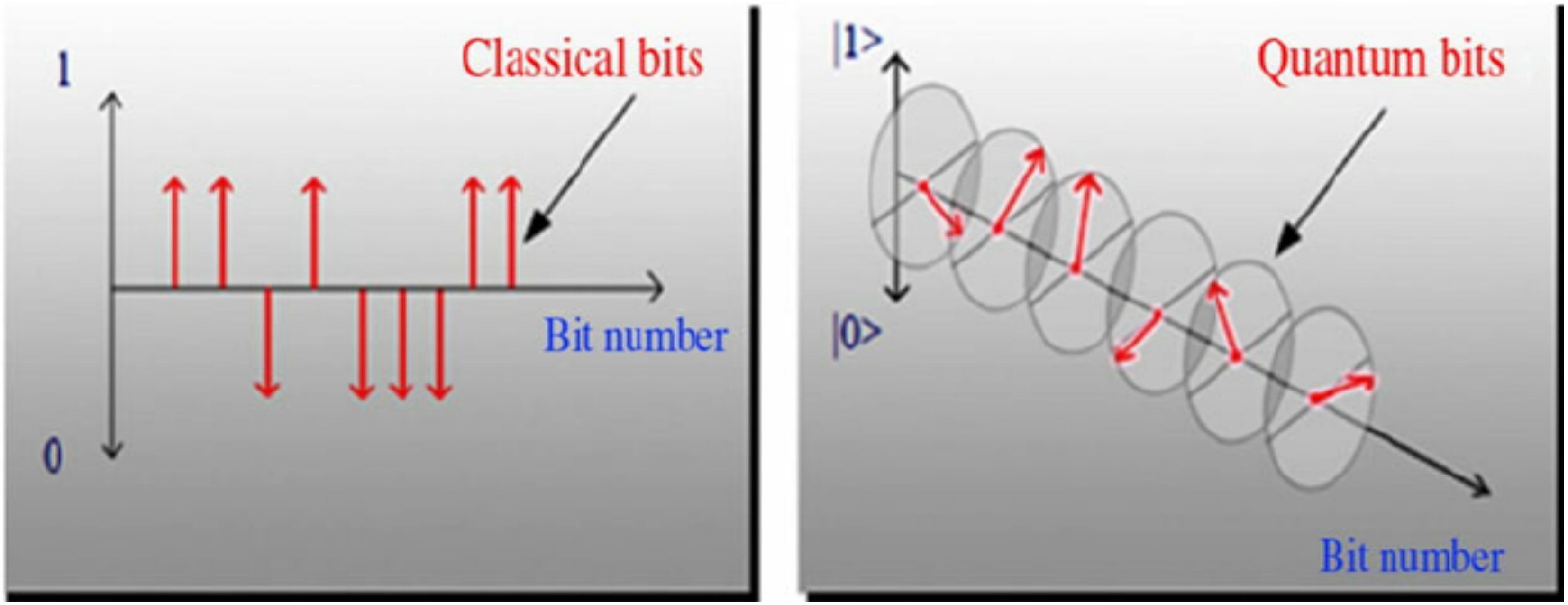
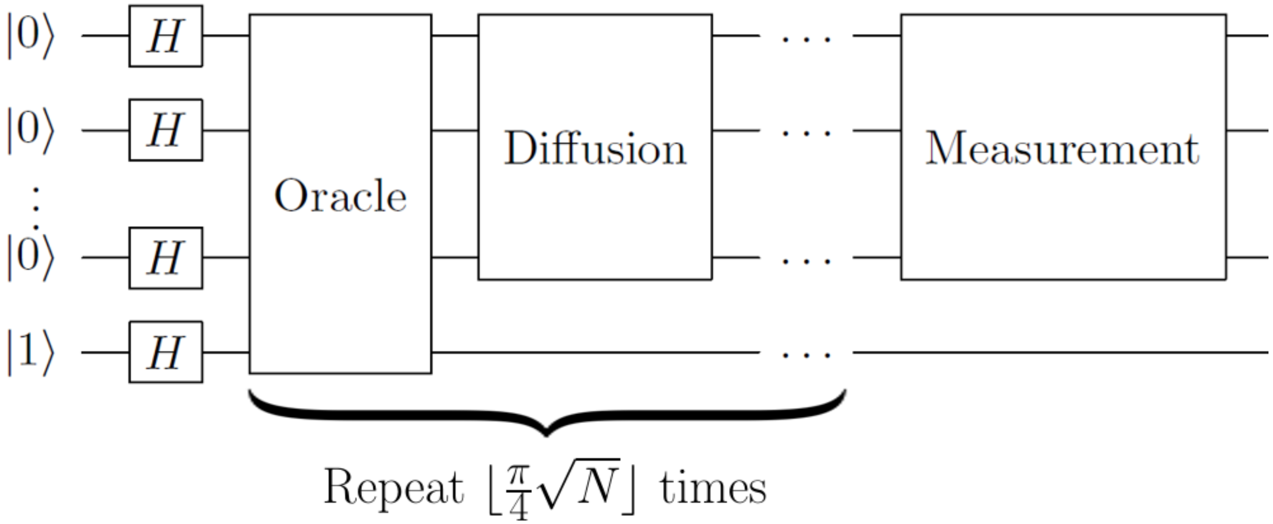
QC in a nutshell



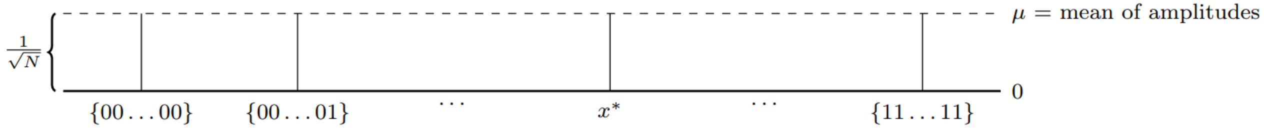
Farouk et al.: Architecture of multicast centralized key management scheme using Quantum key distribution and classical symmetric encryption (2014)

Grover's search algorithm



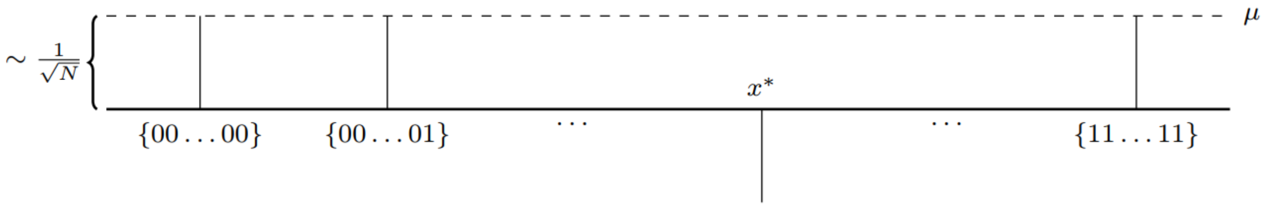
v.d. Lans: QAs and their implementation on QC simulators (2017)

Grover's search algorithm



Wright, Tseng: Grover's algorithm (2015)

Grover's search algorithm



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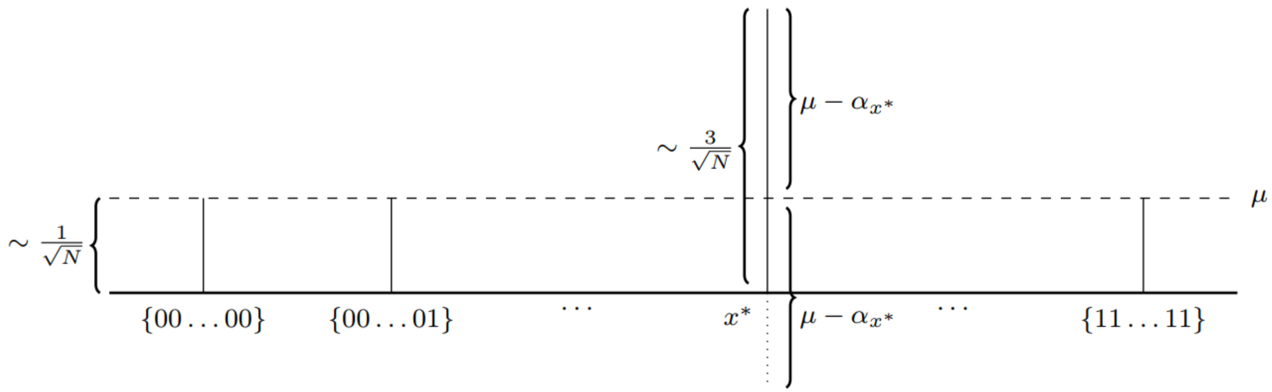

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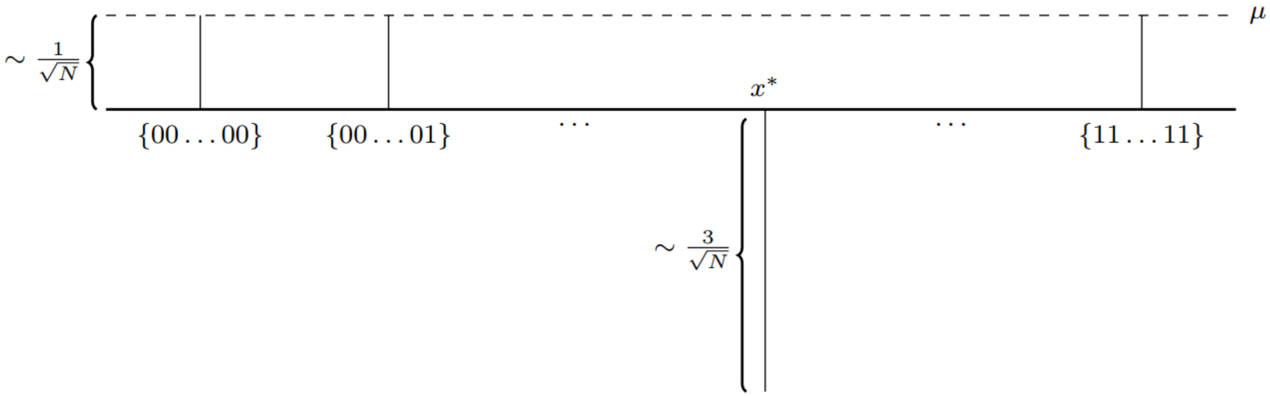

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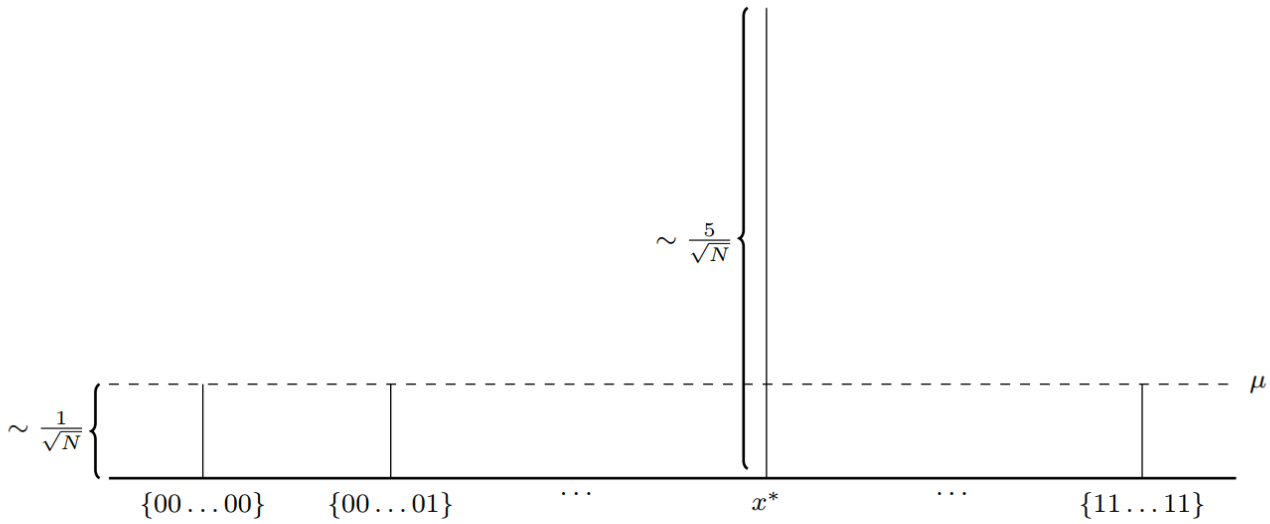
Grover’s search algorithm



Wright, Tseng: Grover’s algorithm (2015)

Long-term vision

Microprocessors and Microsystems 66 (2019) 67–71

Contents lists available at ScienceDirect

Microprocessors and Microsystems

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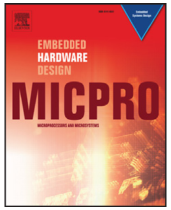

A conceptual framework for quantum accelerated automated design optimization

Check for updates

Matthias Möller[a,*], Cornelis Vuik[a]

Delft University of Technology, Delft Institute of Applied Mathematics (DIAM), Van Mourik Broekmanweg 6, XE Delft 2628, The Netherlands

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Design optimization

- **Abstract problem**:

$$\min_{\boldsymbol{\alpha}\in\mathcal{D}} \mathcal{J}(U(\boldsymbol{\alpha}); Y) \quad \text{s.t.} \quad \mathcal{R}(U(\boldsymbol{\alpha}); Y) = 0$$

  - Admissible design parameters $\boldsymbol{\alpha} \in \mathcal{D}$
  - Generated design (control) $U(\boldsymbol{\alpha})$
  - Solution $Y = Y(U(\boldsymbol{\alpha}))$ to PDE in residual form
  - Cost functional $\mathcal{J}(\cdot)$ to be minimized

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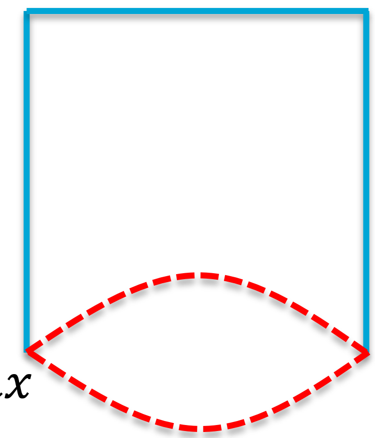
Academic model problem

- **2D Poisson equation**:

$$
\begin{aligned}
-\Delta u &= f \text{ in } \Omega(\alpha) \\
u &= 0 \text{ on } \Gamma(\alpha)
\end{aligned}
$$

- **Design parameter**:

$$y(x) = \alpha(x - x^2), \alpha^{min} \leq \alpha \leq \alpha^{max}$$



- **Optimization problem**:
  - Minimize L_2-error between solution u and a given reference profile u^* by adjusting the shape of the domain boundary at the bottom

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Q-accelerated linear solvers

- **Discretized problem**:

$$\min_{\alpha \in \mathcal{D}} \left(\int_{\Omega(\alpha)} y_h^2 \, dx \right)^{\frac{1}{2}} \approx \min_{\alpha \in \mathcal{D}} \left(y_h^T M y_h \right)^{\frac{1}{2}}$$

sparse matrix

such that

s-sparse SPD well-conditioned matrix

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

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Q-accelerated optimization

- **Taylor expansion about the optimal state $\boldsymbol{\alpha}^*$:**

$$\mathcal{J}\left(\boldsymbol{\alpha}^{(k)}\right) - \mathcal{J}(\boldsymbol{\alpha}^*) =$$

$$\cancel{\sum_{i=1}^{\dim \mathcal{D}} \left.\frac{\partial \mathcal{J}}{\partial \alpha_i}\right|_{\boldsymbol{\alpha}^*} \left(\alpha_i^{(k)} - \alpha_i^*\right)}$$

$$+\frac{1}{2}\sum_{i,j=1}^{\dim \mathcal{D}} \left(\alpha_i^{(k)} - \alpha_i^*\right) \left.\frac{\partial^2 \mathcal{J}}{\partial \alpha_i \partial \alpha_j}\right|_{\boldsymbol{\alpha}^*} \left(\alpha_i^{(k)} - \alpha_i^*\right)$$

$$+\mathcal{O}\left(\left\|\boldsymbol{\alpha}^{(k)} - \boldsymbol{\alpha}^*\right\|^3\right)$$

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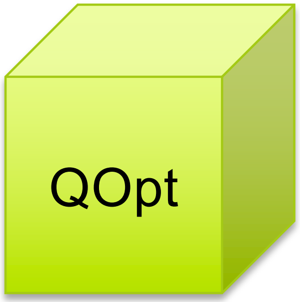
Q-accelerated optimization

- **Positive-definite quadratic form**:

$$\mathcal{Q}\left(\boldsymbol{\alpha}^{(k)}\right) = \frac{1}{2} \sum_{i,j=1}^{\dim \mathcal{D}} \left(\alpha_i^{(k)} - \alpha_i^*\right) \frac{\partial^2 \mathcal{J}}{\partial \alpha_i \partial \alpha_j}\bigg|_{\boldsymbol{\alpha}^*} \left(\alpha_i^{(k)} - \alpha_i^*\right)$$



Potential Q-speedup

- **QLSA**:
  - CG method: $\mathcal{O}(N s\kappa \log(1/\epsilon))$
  - HHL (2009): $\mathcal{O}(\log(N) s^2\kappa^2/\epsilon)$
  - Ambainis (2012): $\mathcal{O}(\log(N) s^2\kappa/\epsilon)$
  - Childs et al. (2017): $\mathcal{O}(\text{polylog}(s\kappa/\epsilon) s\kappa)$

- **QOpt**:
  - Yao (1975): $\mathcal{O}(\dim \mathcal{D}^2)$
  - Jordan (2008): $\mathcal{O}(\dim \mathcal{D})$

- **Other**:
  - Cao et al. (2013): FDM Q-Poisson solver
  - Montanaro et al. (2016): FEM Q-Poisson solver

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Surrogate modelling of PDEs
Aircraft Loading Optimization
Airbus Quantum Computing Challenge
Bringing flight physics into the Quantum Era

Wrap-up

- **LibKet:**
  - Early adopter usage and feedback highly appreciated
- **Q-accelerated shape optimization**:
  - Feedback on concept and collaboration welcome
- **Possible collaboration with NLR**:
  - Airbus Quantum Challenge and other topics
  - Q-Flagship project (coordinated by K. Bertels)

Thank you for your attention!

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