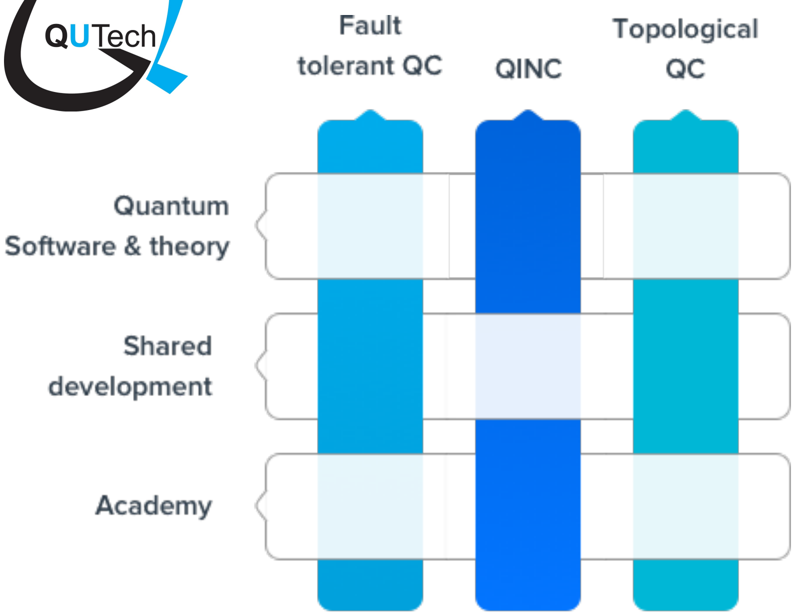
A conceptual framework for structural design and optimization using quantum computing

Matthias Möller
Assistant Professor, Numerical Analysis
Delft University of Technology
Delft Institute of Applied Mathematics

Quantum Computing at TU Delft

QuTech



Quantum & Computer Engineering

Delft
Institute of
Applied
Mathematics

Quantum Computing at DIAM

- Bachelor projects
  - M. v.d. Lans: Multi-search Groover, Q-add/sub
  - M. Looman: Q-add with simulated quantum errors
  - R. Nugteren: Q-mul for Noisy Intermediate-Scale Quantum (NISQ)
  - S. v.d. Linde: Posit arithmetics
  - O. Ubbes: Quantum Linear Solver Algorithm (QLSA)
  - T. Driebergen: Posit arithmetics for QC
  - M. Schalkers (internship at TNO): LibKet, unitary decomposition

- Collaborations and support:
  - TNO, TU Delft Quantum & Computer Engineering, SURFsara, 4TU.CEE

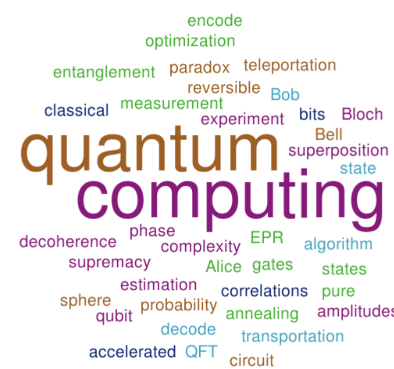
Outlook

- Basic Concepts of quantum computing
  - *Quantum bits, registers, gates, and algorithms*

- Quantum-accelerated design optimization
  - *A conceptual framework*

- Practical aspects of quantum computing
  - *SDKs and good practices*

- Conclusion

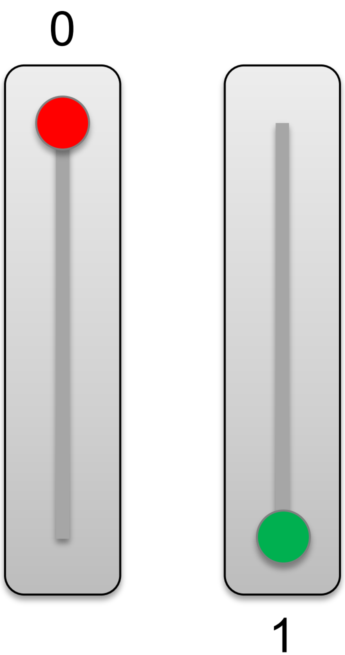


Basic concepts of quantum computing

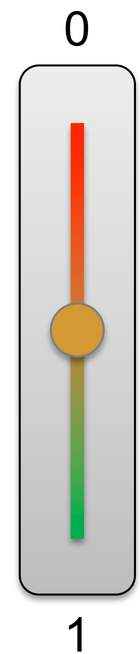
QUANTUM BITS

From bits to quantum bits

- Classical bits

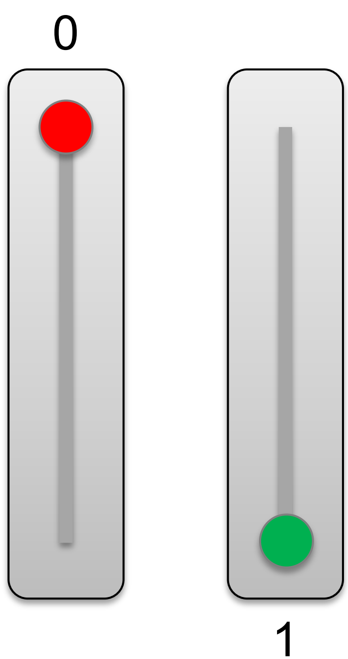


- Quantum bits (qubits)

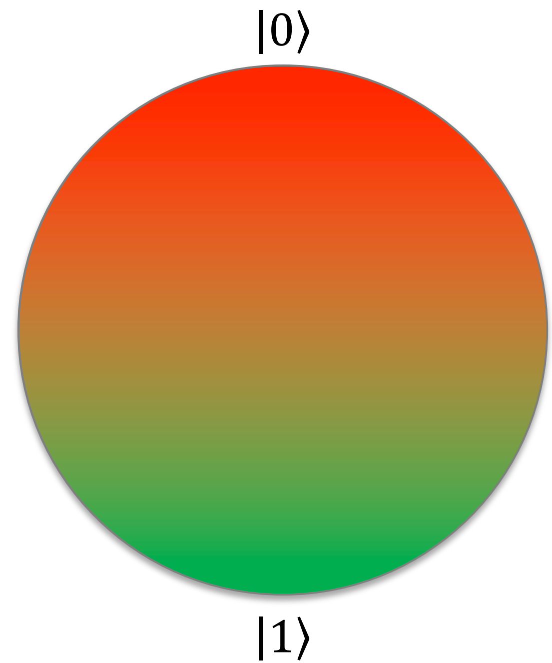


From bits to quantum bits

- Classical bits



- Quantum bits (qubits)

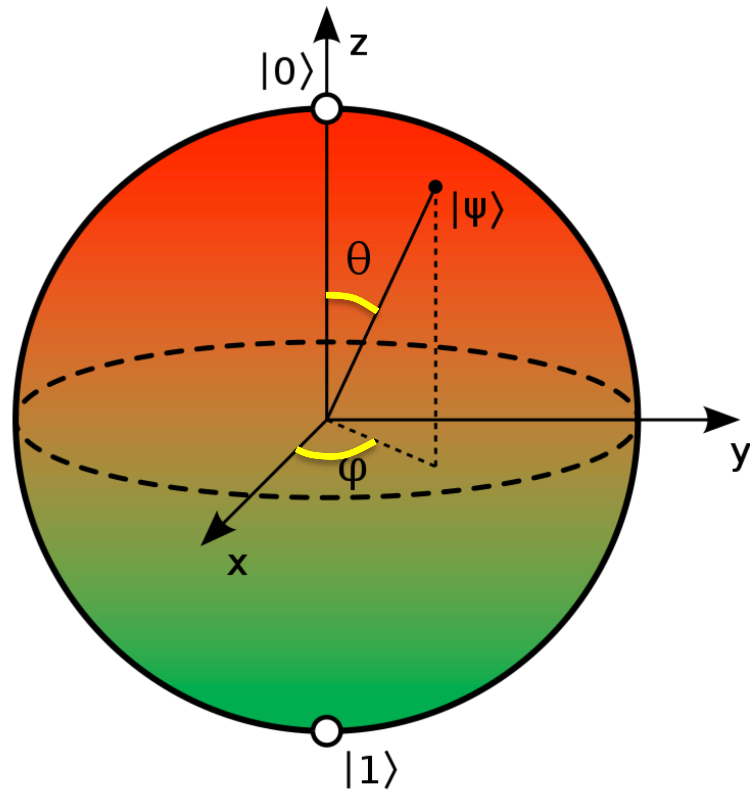


The Bloch sphere

- Quantum state

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

- Basis states $|0\rangle$ and $|1\rangle$
- Latitude $\theta \in [0, \pi]$
- Longitude $\varphi \in [0,2\pi)$



The Bloch sphere, cont'd

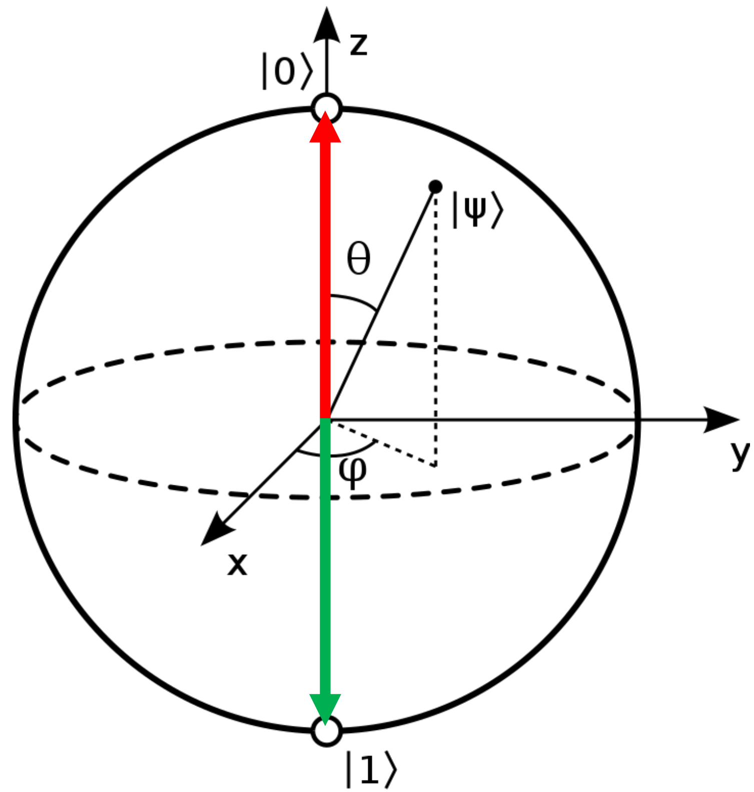
- $\theta = 0$ implies

  $|\psi\rangle = 1 \cdot |0\rangle + e^{i\varphi} \cdot 0 \cdot |1\rangle = |0\rangle$

- $\theta = \pi$ implies

  $|\psi\rangle = 0 \cdot |0\rangle + e^{i\varphi} \cdot 1 \cdot |1\rangle = |1\rangle$

- *Poles represent classical bits*



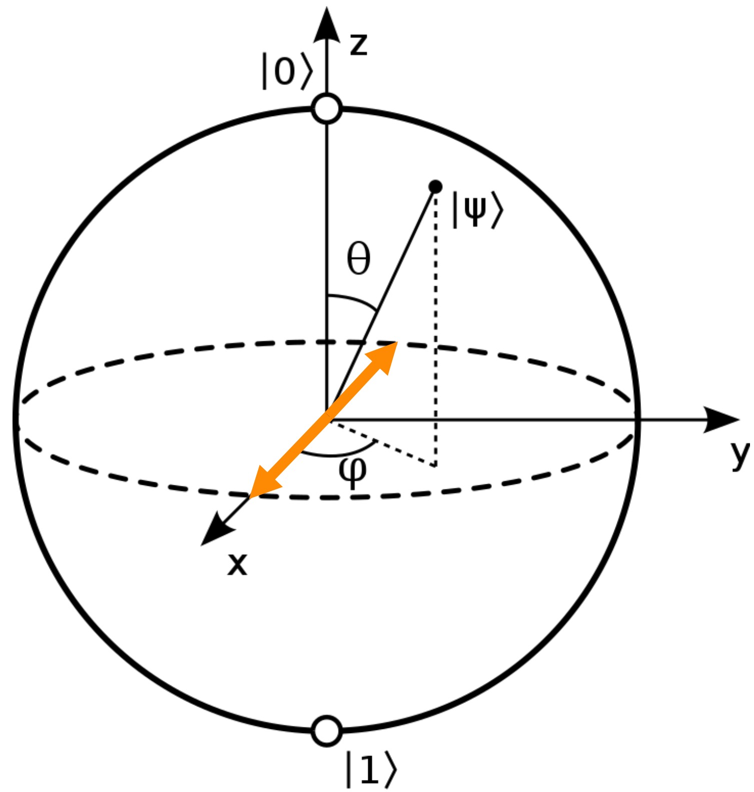
The Bloch sphere, cont'd

- $\theta = \frac{\pi}{2}$ and $\varphi = 0$ implies

$$|\psi\rangle = \frac{1}{\sqrt{2}} \cdot |0\rangle + \frac{e^{i0}}{\sqrt{2}} \cdot |1\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

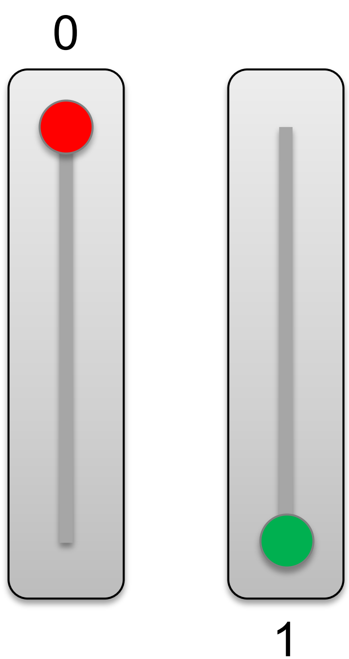
- $\theta = \frac{\pi}{2}$ and $\varphi = \pi$ implies

$$|\psi\rangle = \frac{1}{\sqrt{2}} \cdot |0\rangle + \frac{e^{i\pi}}{\sqrt{2}} \cdot |1\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

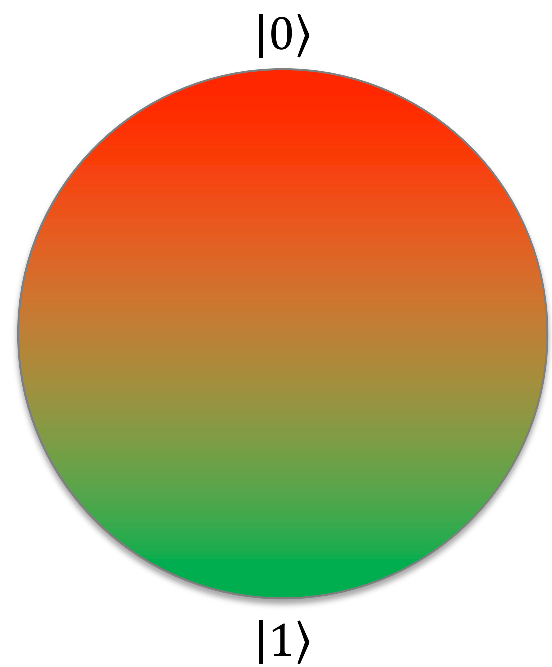


What to do with this added value?

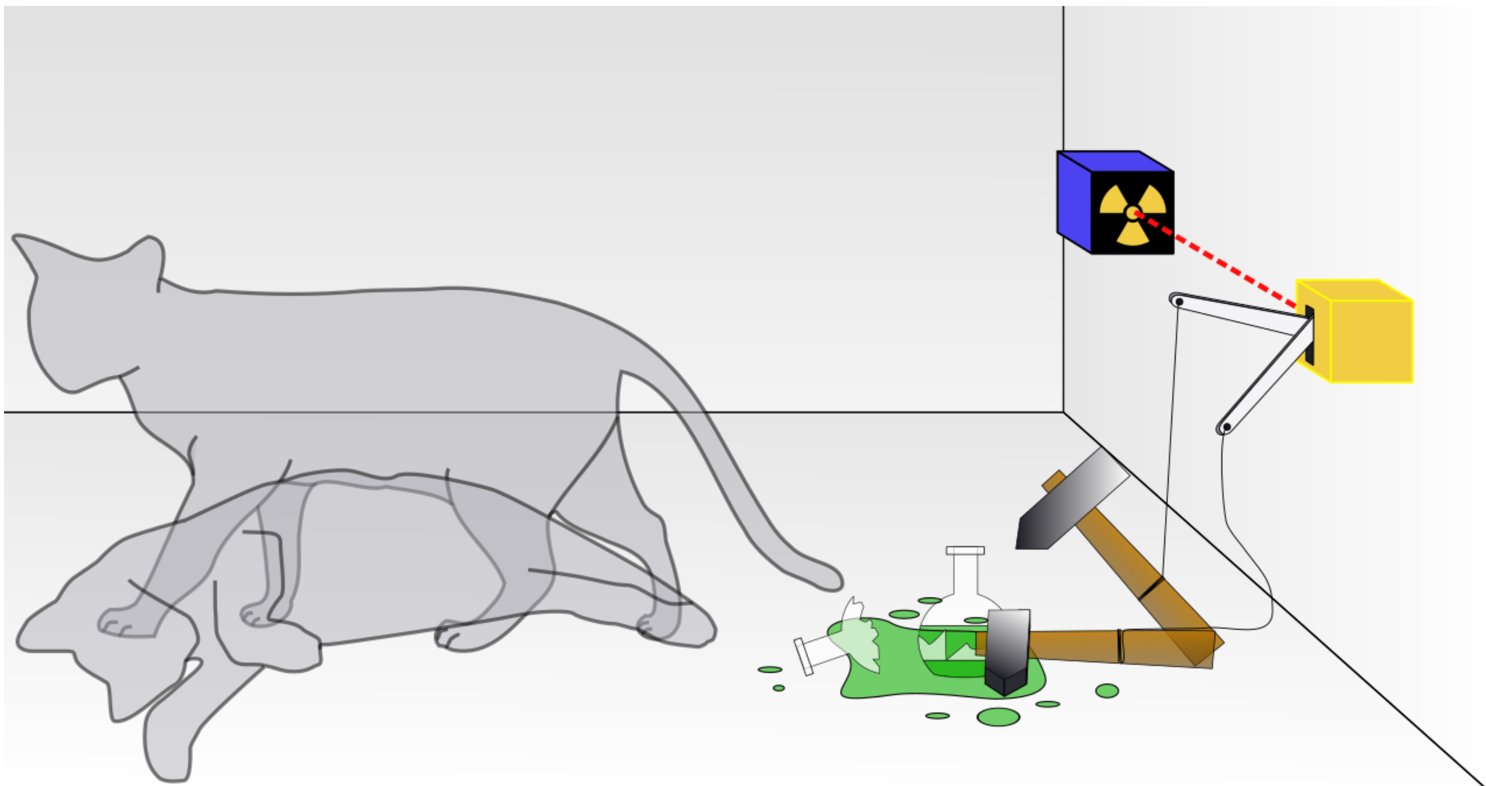
- Classical bits



- Quantum bits (qubits)

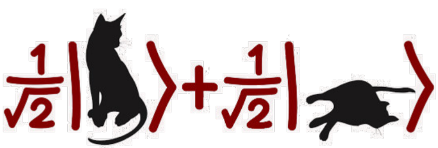


Intermezzo: Schrödinger's cat



Intermezzo: Schrödinger’s cat, cont’d

- Before opening the box

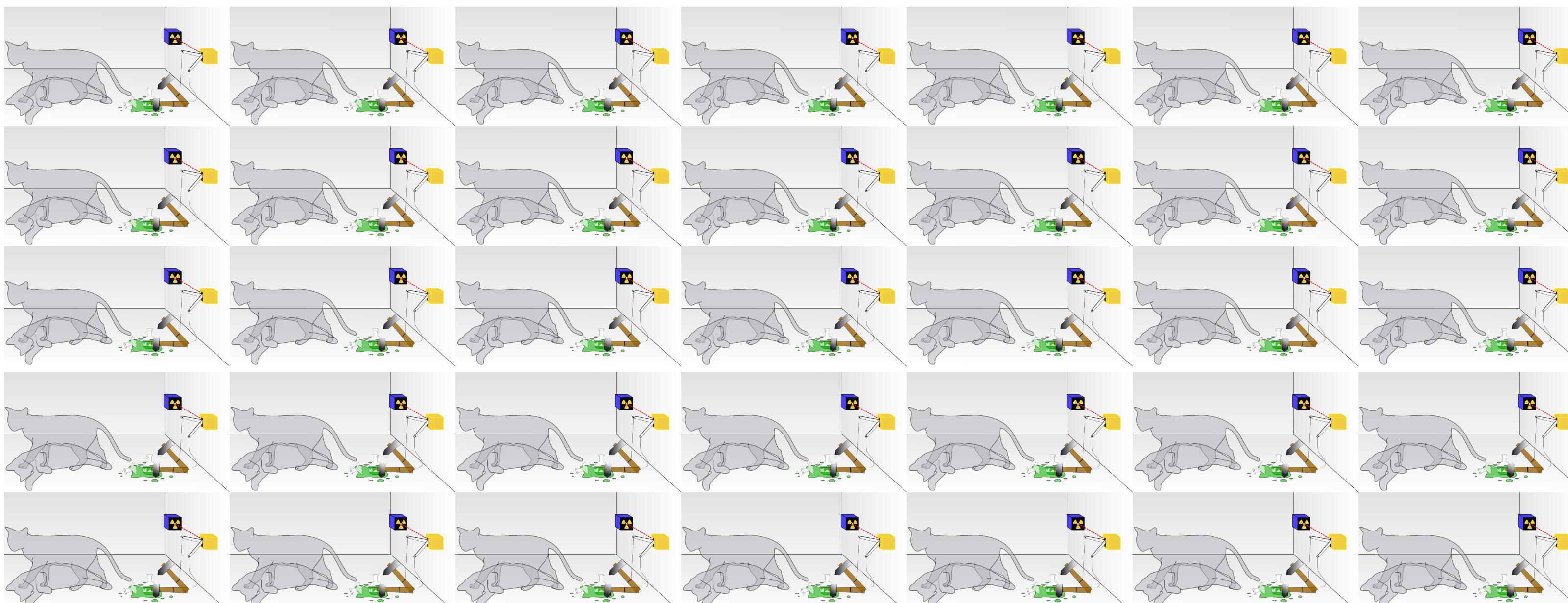


- After opening the box

OR

Intermezzo: Schrödinger's cat, cont'd

- Repeating the experiment many times 50% of the cats are dead, 50% alive



From Bloch's sphere to probabilities

- Coefficients of the basis expansion

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

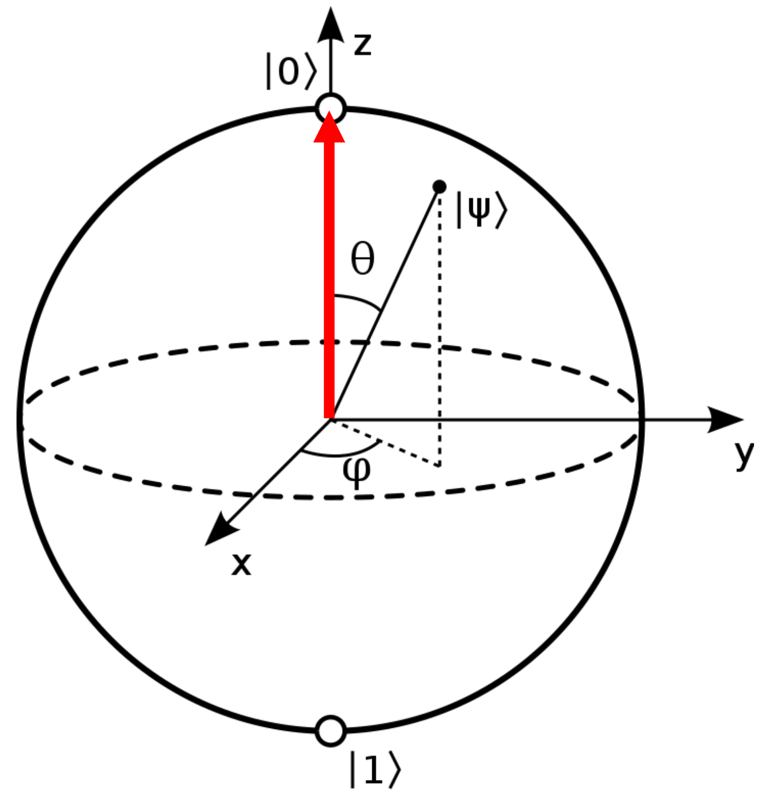
represent the probability amplitude that the quantum state $|\psi\rangle$ collapses to either of the two basis states $|0\rangle$ or $|1\rangle$ upon measurement since

$$\left|\cos\frac{\theta}{2}\right|^2 + \left|e^{i\varphi} \cdot \sin\frac{\theta}{2}\right|^2 = 1$$

for all latitudes $\theta \in [0, \pi]$ and longitudes $\varphi \in [0,2\pi)$

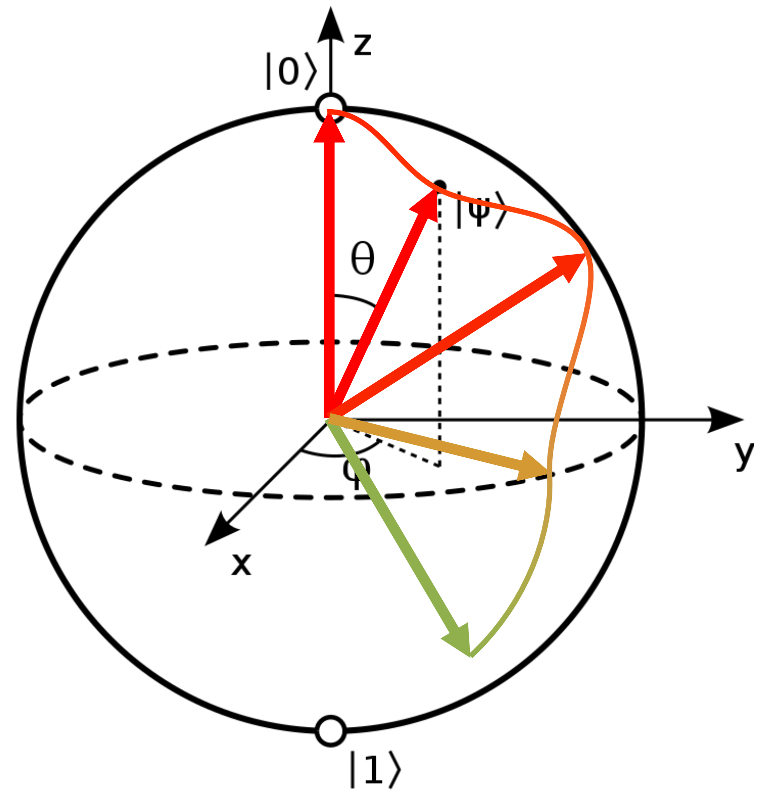
Life of a qubit

- Initialization into pure state $|0\rangle$



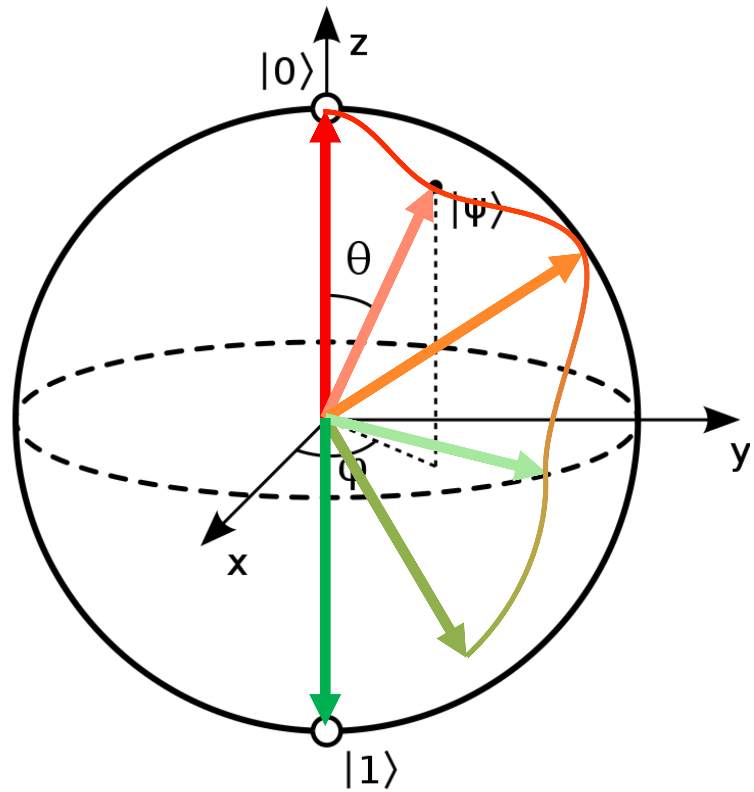
Life of a qubit

- Initialization into pure state $|0\rangle$
- Travelling on Bloch's sphere



Life of a qubit

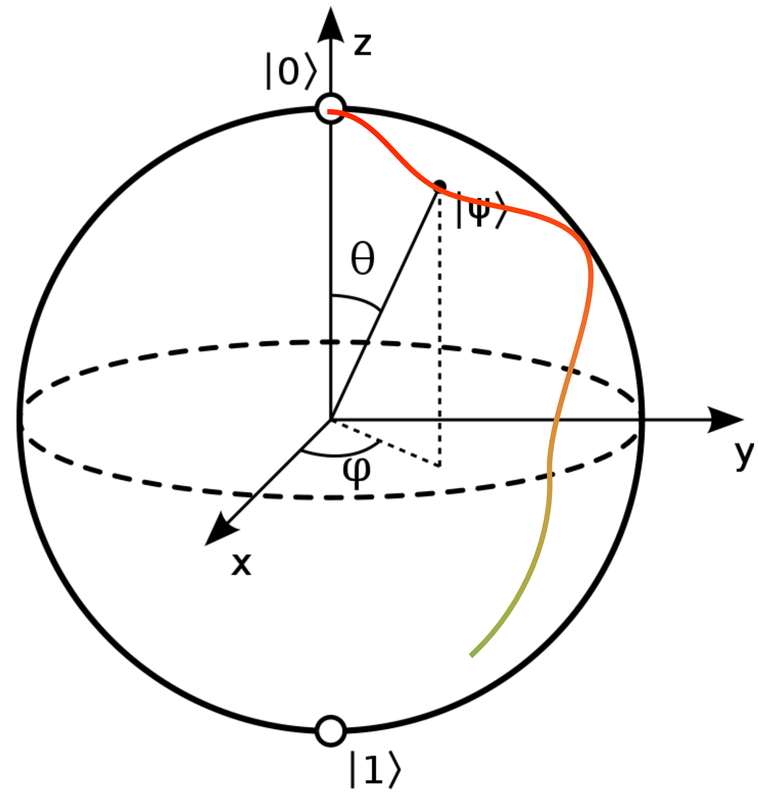
- Initialization into pure state $|0\rangle$
- Travelling on Bloch's sphere
- Collapsing to either $|0\rangle$ or $|1\rangle$



Life of a qubit

- Initialization into pure state $|0\rangle$
- Travelling on Bloch's sphere
- Collapsing to either $|0\rangle$ or $|1\rangle$

- *How to describe the travelling?*



Basic concepts of quantum computing

QUANTUM GATES

Detour to linear algebra

- Standard basis for a single-qubit state

$$E = (|0\rangle, |1\rangle) \quad with \quad \begin{pmatrix} 1 \\ 0 \end{pmatrix} := |0\rangle, \qquad \begin{pmatrix} 0 \\ 1 \end{pmatrix} := |1\rangle$$

- Probability amplitudes (= the coefficients $|\psi\rangle$ of w.r.t. to basis E)

$$\alpha_0 := \cos\frac{\theta}{2}, \qquad \alpha_1 := e^{i\varphi} \cdot \sin\frac{\theta}{2}$$

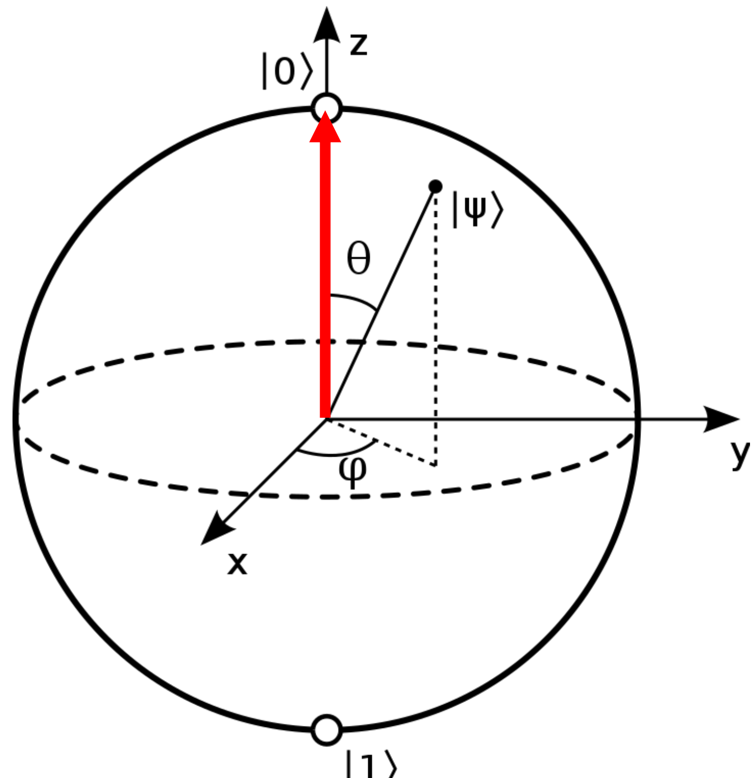
- Coordinate representation

$$|\psi\rangle = \alpha_0 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \alpha_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow [|\psi\rangle]_E = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix}$$

Detour to linear algebra, cont'd

- Initialization into pure state

$$|\psi\rangle = 1 \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + 0 \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$



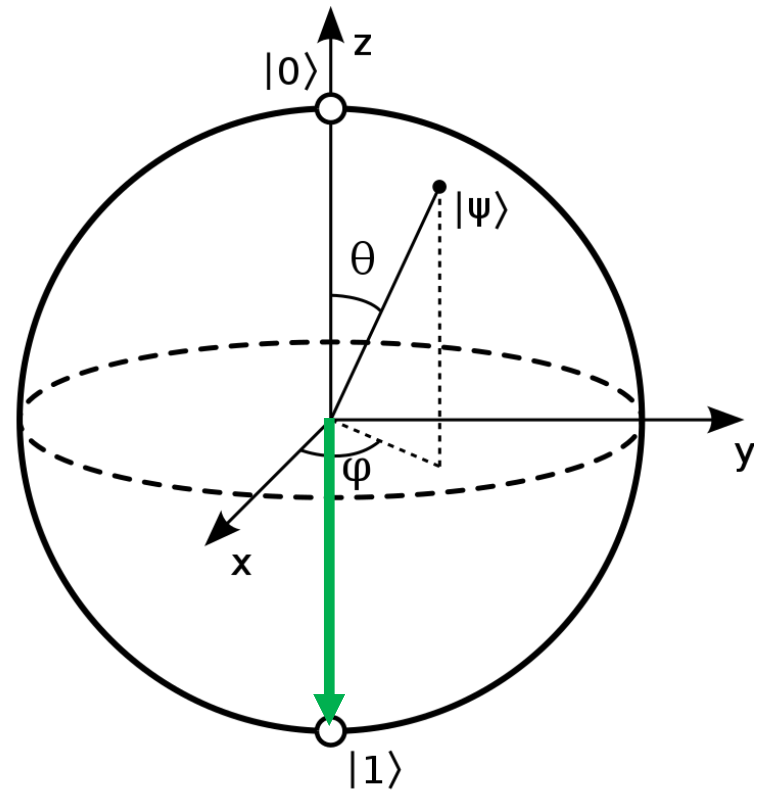
Detour to linear algebra, cont'd

- Initialization into pure state

$$|\psi\rangle = 1 \cdot \begin{pmatrix}1\\0\end{pmatrix} + 0 \cdot \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}1\\0\end{pmatrix}$$

- Multiplication with X

$$X \cdot |\psi\rangle \coloneqq \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} \cdot \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\\1\end{pmatrix}$$



Detour to linear algebra, cont'd

- Initialization into pure state

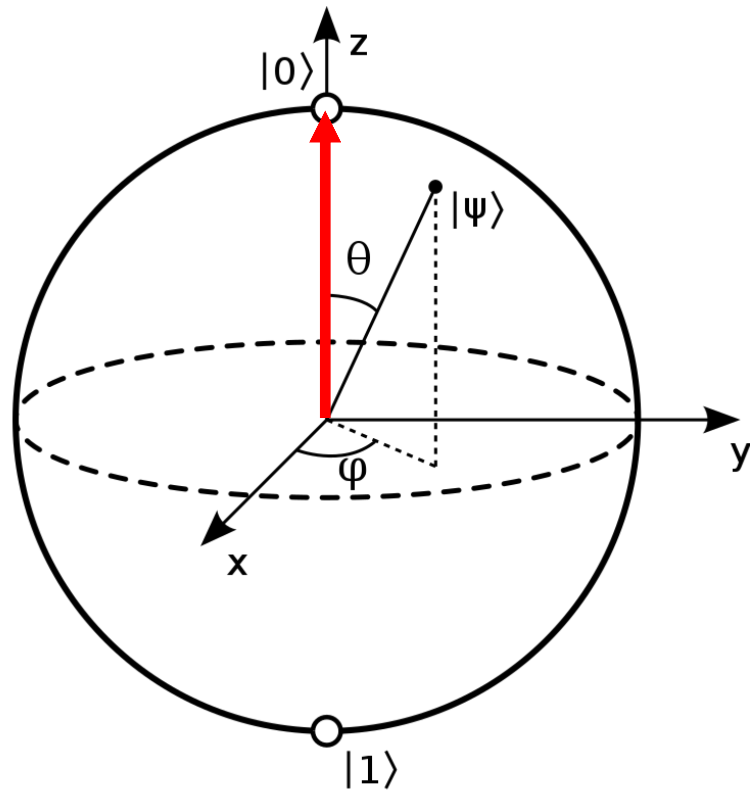
$$|\psi\rangle = 1 \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + 0 \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

- Multiplication with X

$$X \cdot |\psi\rangle \coloneqq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

- Multiplication with X once more

$$X \cdot X \cdot |\psi\rangle \coloneqq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$



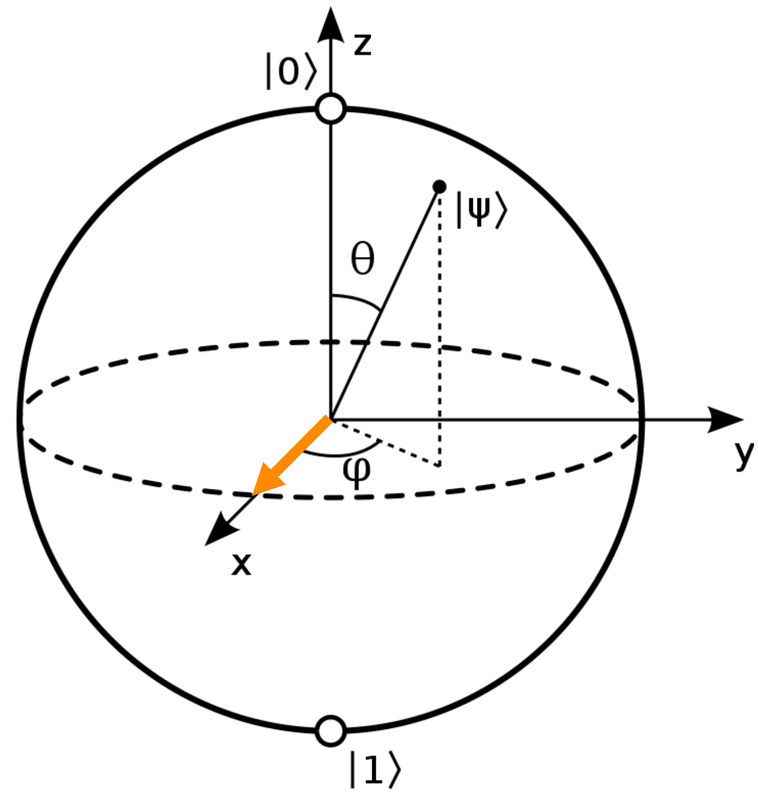
Detour to linear algebra, cont'd

- Initialization into pure state

$$|\psi\rangle = 1 \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + 0 \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

- Multiplication with another matrix

$$H \cdot |\psi\rangle := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$



Detour to linear algebra, cont'd

- Initialization into pure state

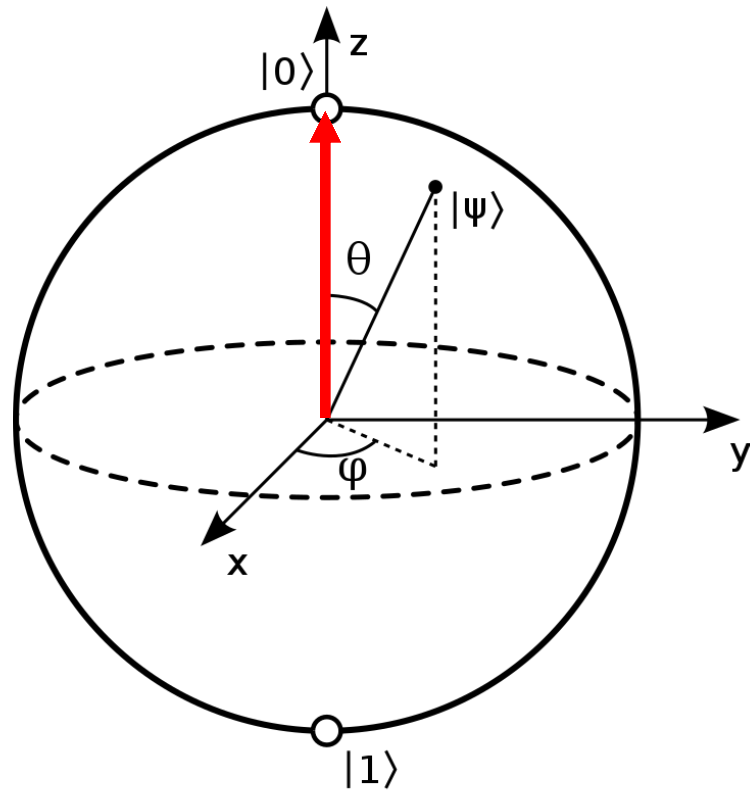
$$|\psi\rangle = 1 \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + 0 \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

- Multiplication with another matrix

$$H \cdot |\psi\rangle \coloneqq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

- Double application of matrix H gives

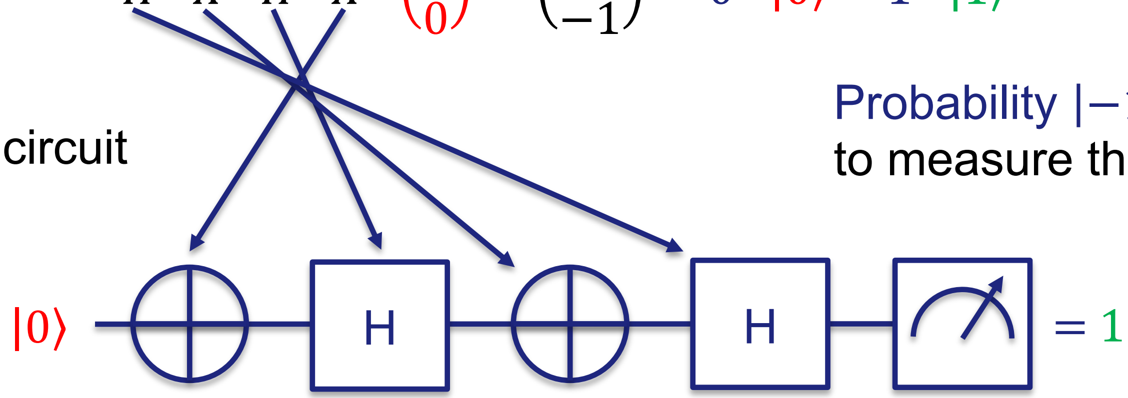
$$H^2 \cdot |\psi\rangle \coloneqq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$



Et voilà, our first quantum algorithm

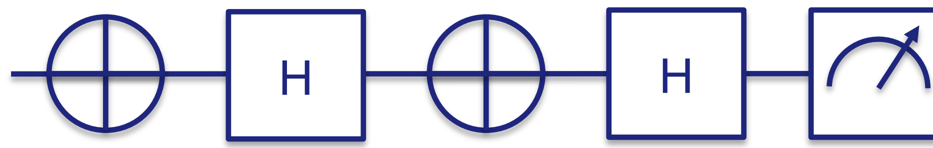
$$H \cdot X \cdot H \cdot X \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} = 0 \cdot |0\rangle - 1 \cdot |1\rangle$$

- Quantum circuit



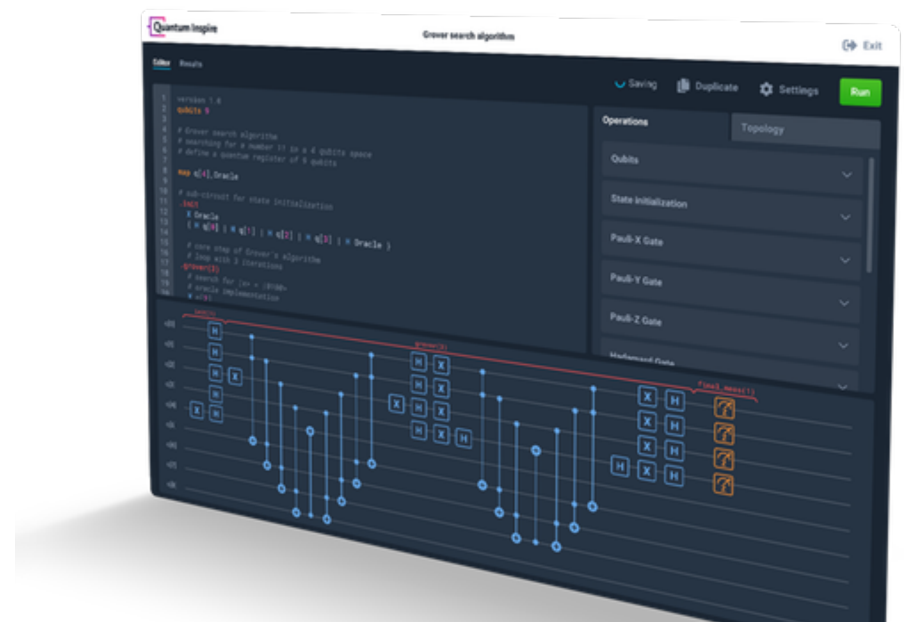
Probability $|-1|^2 = 1$
to measure the 1 state

Quantum Inspire




```
version 1.0

qubits 1
prep_z q[0]
X q[0]
H q[0]
X q[0]
H q[0]
measure q[0]
```



quantum-inspire.com

Detour to linear algebra, again

- Quantum gates can be expressed as **unitary matrices**
  - $U \cdot U^{\dagger} = I = U^{\dagger} \cdot U$ (quantum gates are reversible)
  - $\forall x \in \mathbb{C}^n, \|Ux\| = \|x\|$ (length is preserved)
  - $\forall x, y \in \mathbb{C}^n, \langle Ux, Uy \rangle = \langle x, y \rangle$ (inner product is preserved)

- Quantum algorithms can be expressed as chains of mat-vec multiplications

$$|\psi_{out}\rangle = U_d \cdot U_{d-1} \cdot \ldots \cdot \underbrace{U_2 \cdot \underbrace{U_1 \cdot |\psi_{in}\rangle}_{|\psi'\rangle}}_{|\psi''\rangle} = {\color{red}U} \cdot |\psi_{in}\rangle$$

Reversible computing

- Quantum algorithms can be easily reversed (in theory!)

$$U_d^\dagger \cdot |\psi_{out}\rangle = \underbrace{U_d^\dagger \cdot U_d}_{I} \cdot U_{d-1} \cdot \ldots \cdot U_2 \cdot U_1 \cdot |\psi_{in}\rangle$$

$$U_{d-1}^\dagger \cdot U_d^\dagger \cdot |\psi_{out}\rangle = \underbrace{U_{d-1}^\dagger \cdot U_{d-1}}_{I} \cdot U_{d-2} \cdot \ldots \cdot U_2 \cdot U_1 \cdot |\psi_{in}\rangle$$

$$U^\dagger \cdot |\psi_{out}\rangle = U_1^\dagger \cdot U_2^\dagger \cdot \ldots \cdot U_{d-1}^\dagger \cdot U_d^\dagger \cdot |\psi_{out}\rangle = |\psi_{in}\rangle$$

- Many ‘nice’ mathematical properties
  - unitary group $U(n)$
  - unitary decomposition,…

Basic concepts of quantum computing

QUANTUM REGISTERS

Detour to linear algebra, yet again

- Tensor-product construction of single-qubit bases

$$|0\rangle \otimes |0\rangle, \quad |0\rangle \otimes |1\rangle, \quad |1\rangle \otimes |0\rangle, \quad |1\rangle \otimes |1\rangle$$

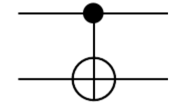
- Unique labelling of multi-qubit state

$$|00\rangle = |0\rangle \otimes |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$|01\rangle = |0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

...

Multiple qubits



$$\begin{bmatrix}1 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 1\\0 & 0 & 1 & 0\end{bmatrix}$$

- Multi-qubit state

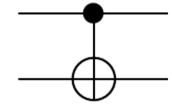
$$|\psi_1\psi_2\rangle = \alpha_0|00\rangle + \alpha_1|01\rangle + \alpha_2|10\rangle + \alpha_3|11\rangle$$

$$= \alpha_0\begin{pmatrix}1\\0\\0\\0\end{pmatrix} + \alpha_1\begin{pmatrix}0\\1\\0\\0\end{pmatrix} + \alpha_2\begin{pmatrix}0\\0\\1\\0\end{pmatrix} + \alpha_3\begin{pmatrix}0\\0\\1\\0\end{pmatrix}$$

- such that

$$|\alpha_0|^2 + |\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2 = 1$$

Multiple qubits, cont'd



$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

- Controlled-NOT gate

$$\mathrm{CNOT}_{12}|\psi_1\psi_2\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_3 \\ \alpha_2 \end{pmatrix}$$

- Outcome

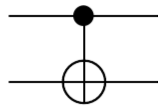
$$\alpha_0|00\rangle + \alpha_1|01\rangle + \alpha_2|10\rangle + \alpha_3|11\rangle$$

$$\mapsto \alpha_0|00\rangle + \alpha_1|01\rangle + \alpha_3|10\rangle + \alpha_2|11\rangle$$

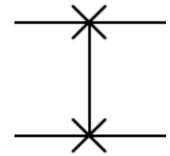
$$= \alpha_0|00\rangle + \alpha_1|01\rangle + \alpha_2|11\rangle + \alpha_3|10\rangle$$

Zoo of quantum gates

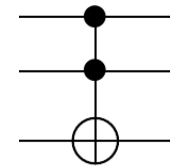
$$\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$$



$$\begin{bmatrix}1 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 1\\0 & 0 & 1 & 0\end{bmatrix}$$

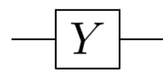


$$\begin{bmatrix}1 & 0 & 0 & 0\\0 & 0 & 1 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 1\end{bmatrix}$$

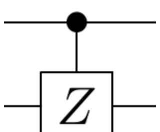


$$\begin{bmatrix}1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\0 & 1 & 0 & 0 & 0 & 0 & 0 & 0\\0 & 0 & 1 & 0 & 0 & 0 & 0 & 0\\0 & 0 & 0 & 1 & 0 & 0 & 0 & 0\\0 & 0 & 0 & 0 & 1 & 0 & 0 & 0\\0 & 0 & 0 & 0 & 0 & 0 & 0 & 1\\0 & 0 & 0 & 0 & 0 & 0 & 1 & 0\end{bmatrix}$$

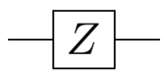
$$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}$$



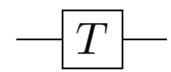
$$\begin{bmatrix}0 & -i\\i & 0\end{bmatrix}$$



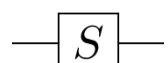
$$\begin{bmatrix}1 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 1 & 0\\0 & 0 & 0 & -1\end{bmatrix}$$



$$\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$$



$$\begin{bmatrix}1 & 0\\0 & e^{i\pi/4}\end{bmatrix}$$

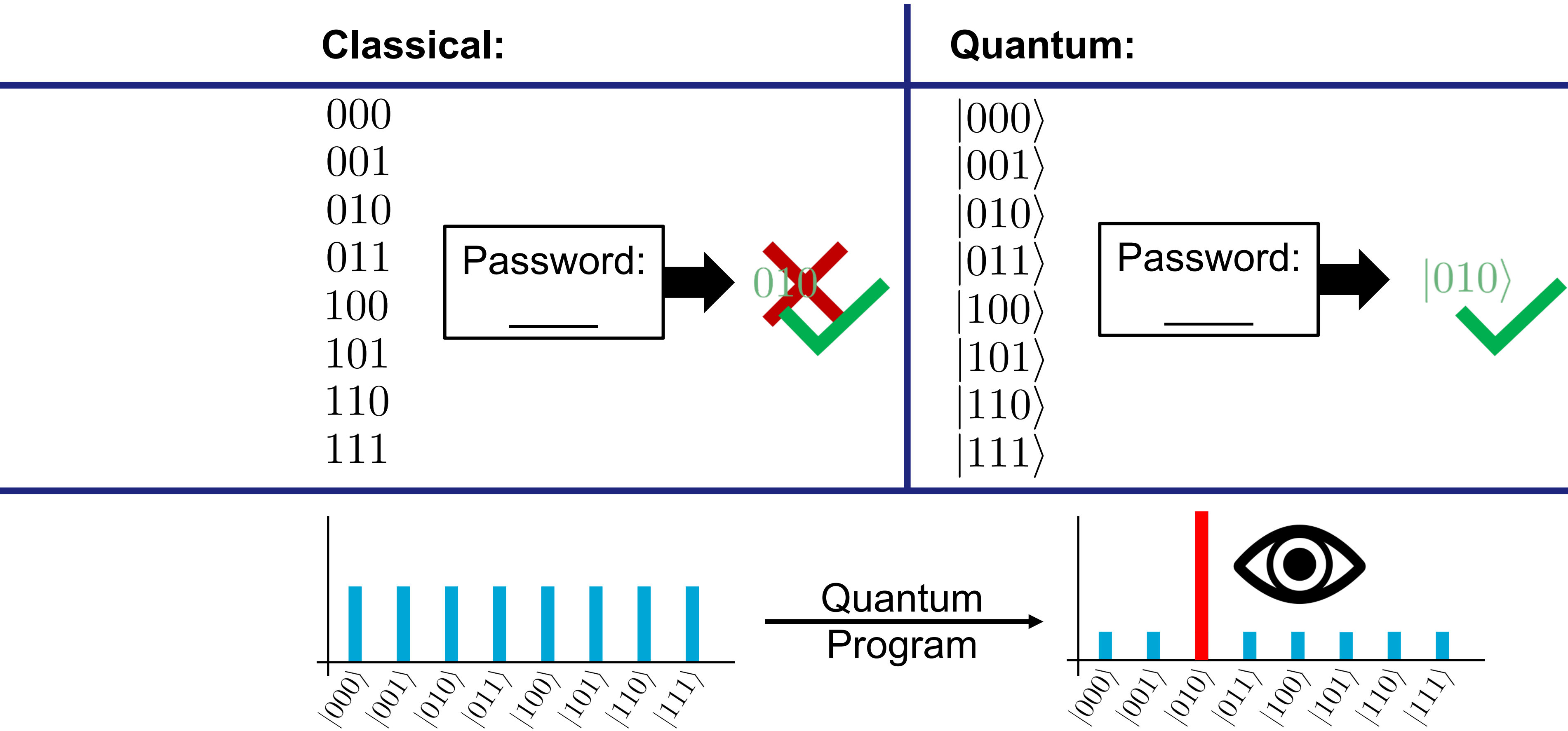


$$\begin{bmatrix}1 & 0\\0 & i\end{bmatrix}$$

Basic concepts of quantum computing

QUANTUM ALGORITHMS

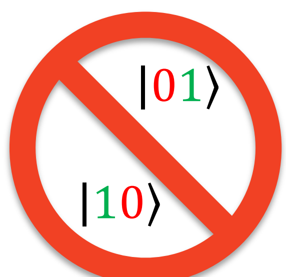
Example: 3-bit password



Bell state

$$|\beta_{00}\rangle = \frac{1}{\sqrt{2}} \cdot |00\rangle + 0 \cdot |01\rangle + 0 \cdot |10\rangle + \frac{1}{\sqrt{2}} \cdot |11\rangle$$

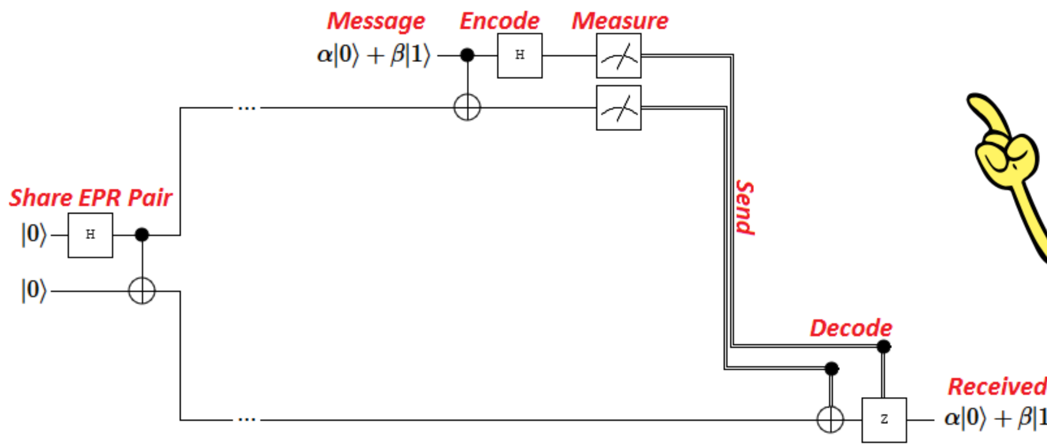
- 50:50 chance to measure $|0?\rangle$ or $|1?\rangle$
- But then we know the value of the second qubit without measurement since

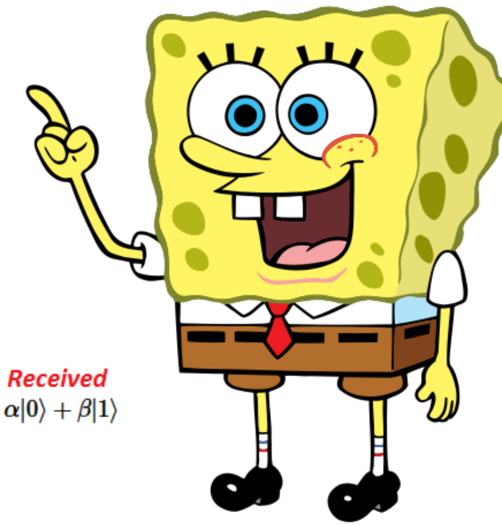


Bell state

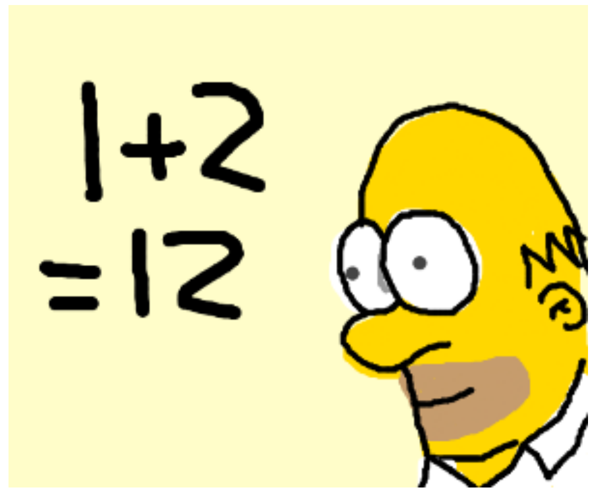
$$|\beta_{00}\rangle = \frac{1}{\sqrt{2}} \cdot |00\rangle + 0 \cdot |01\rangle + 0 \cdot |10\rangle + \frac{1}{\sqrt{2}} \cdot |11\rangle$$

Quantum Teleportation

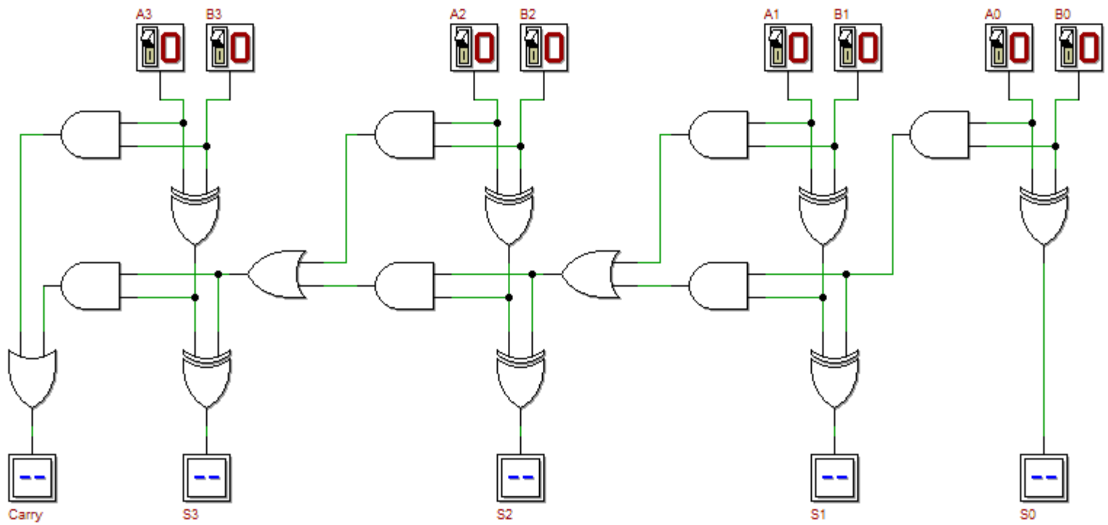




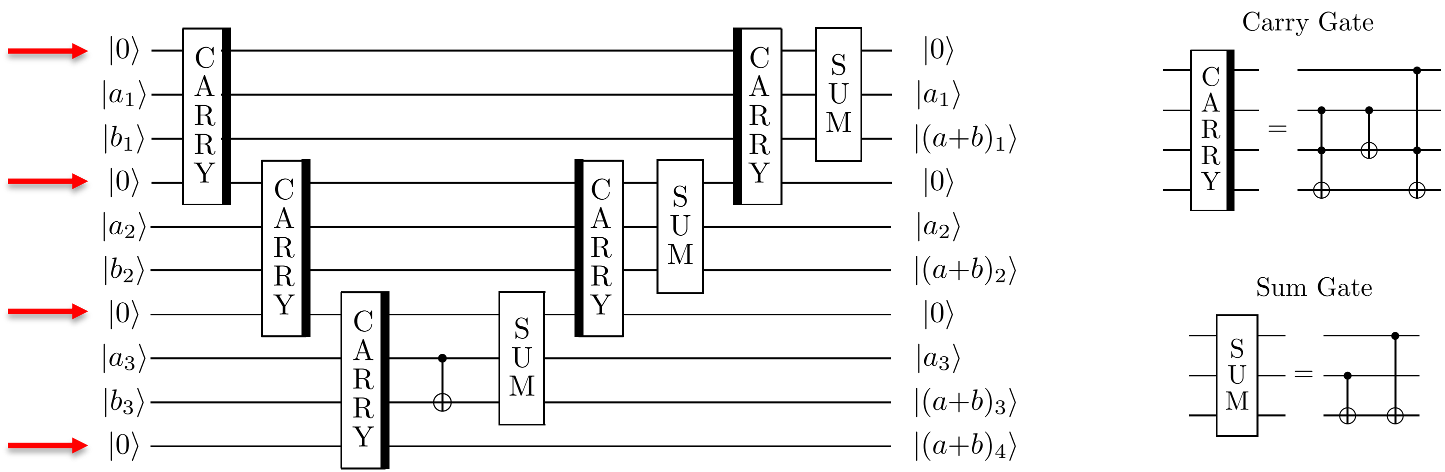
Intermezzo: How difficult can it be to add two integers?



Intermezzo: How difficult can it be to add two integers?



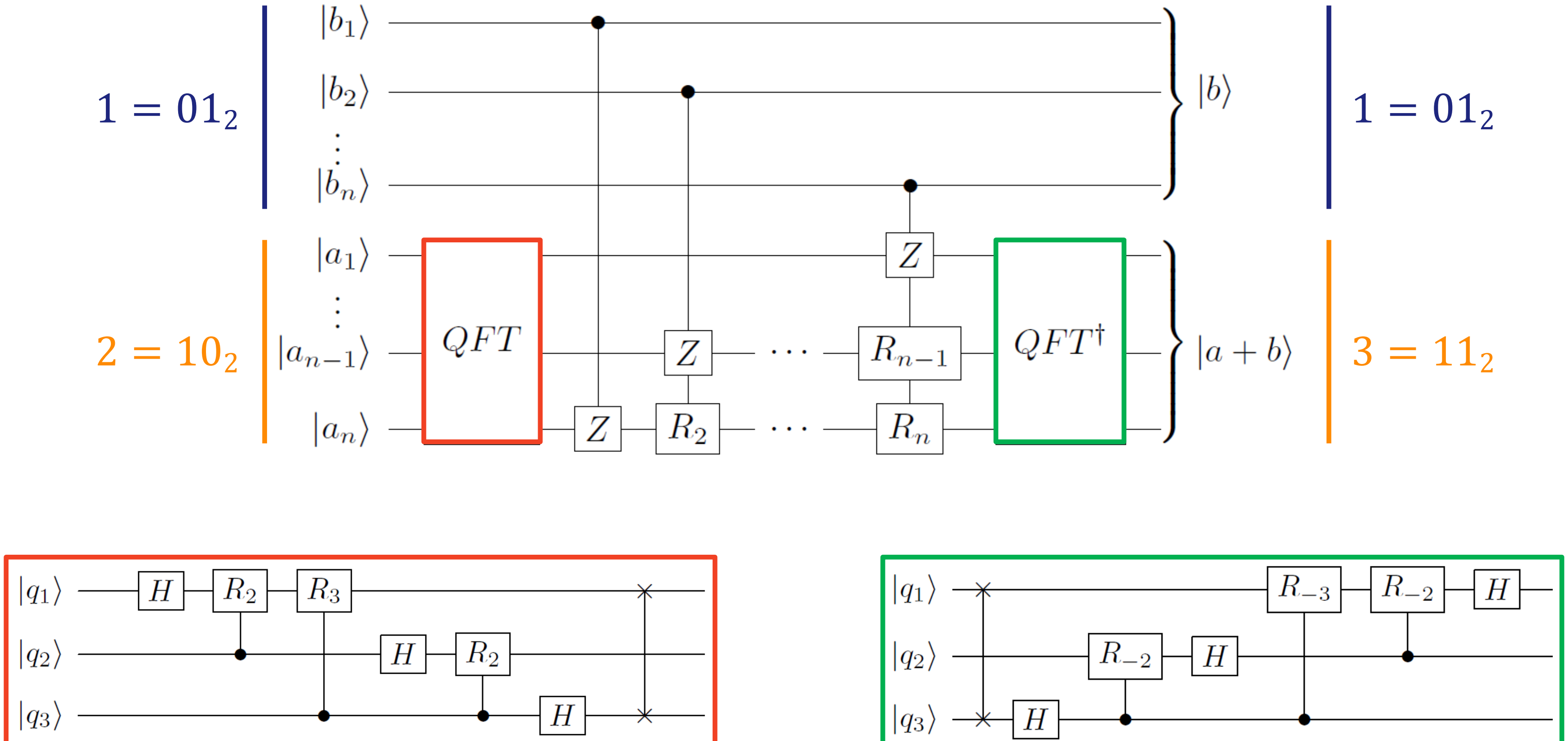
A first quantum algorithm: 1+2=3



n extra ancilla qubits needed ☹

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

Another quantum algorithm: 1+2=3



M. vd. Lans: Quantum Algorithms and their Implementation on Quantum Computer Simulators, Master thesis, 2017

Towards practical QC: 1+2 ≅ 3

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+2 ≅ 3

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

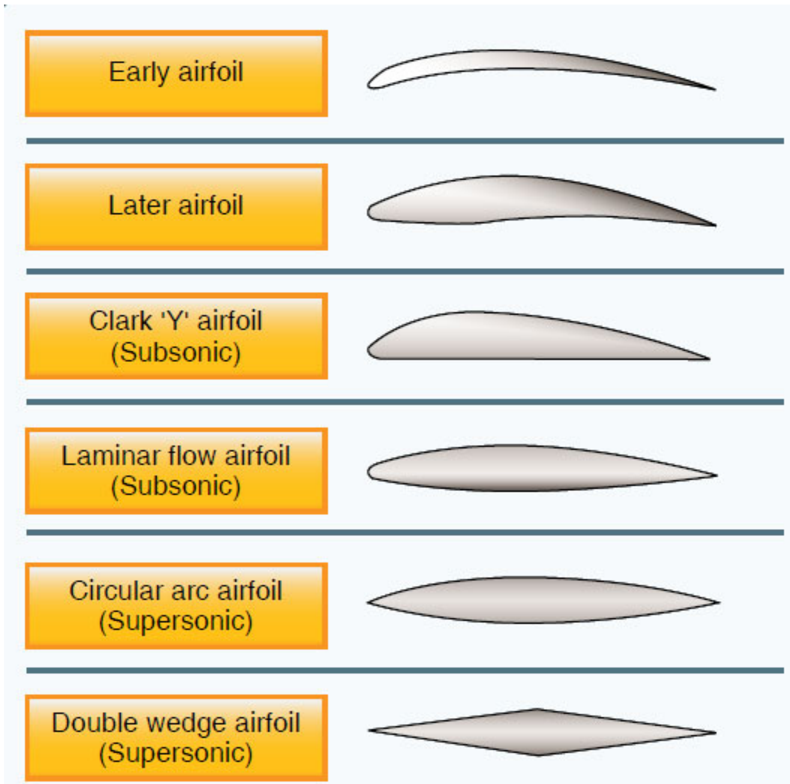
Optimized circuit: prob. correct (left), largest prob. wrong answer (right)

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

Quantum-accelerated design optimization

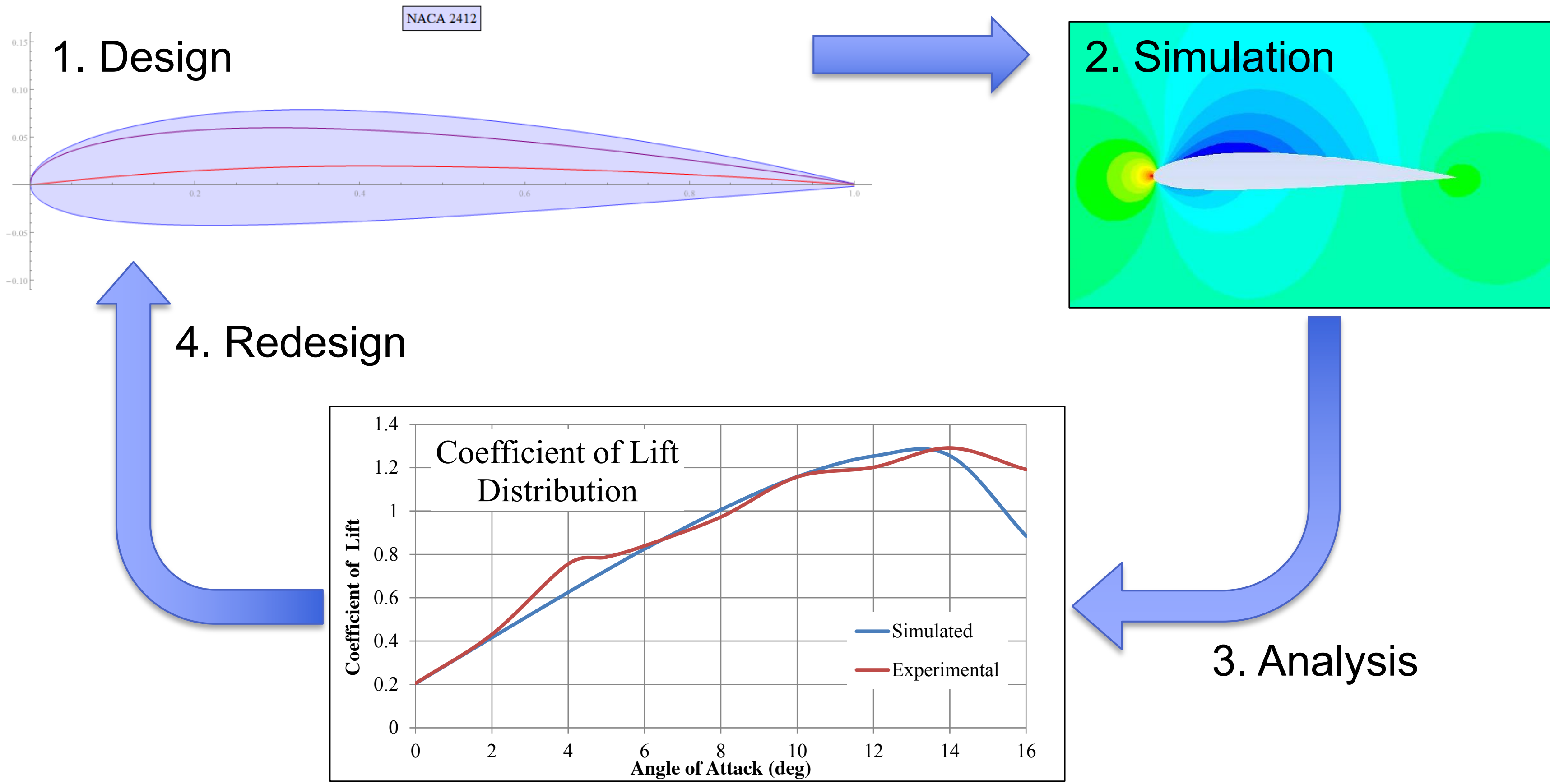
CONCEPTUAL FRAMEWORK

Airfoil design



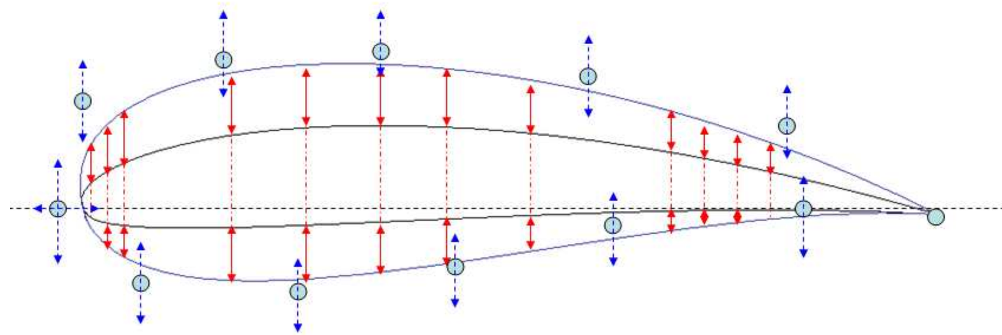
CFInotebook.net

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

1. Design $D(\boldsymbol{p})$



- Design parameters

$$\boldsymbol{p} = (p_1, \dots, p_{12})$$

- Admissible design space

$$\mathcal{S} = [p_1^{min}, p_1^{max}] \times \cdots \times [p_{12}^{min}, p_{12}^{max}]$$

Mauclère, Automatic 2D Airfoil Generation, Evaluation and Optimisation using MATLAB and XFOIL, Master thesis, 2009

2. Simulation

- Mathematical model

Navier-Stokes Equations
3 – dimensional – unsteady

Glenn Research Center

Coordinates: (x,y,z)	Time : t Pressure: p	Heat Flux: q
Velocity Components: (u,v,w)	Density: ρ Stress: τ	Reynolds Number: Re
	Total Energy: Et	Prandtl Number: Pr

Continuity:
$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$$

X – Momentum:
$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} = -\frac{\partial p}{\partial x} + \frac{1}{Re_r}\left[\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z}\right]$$

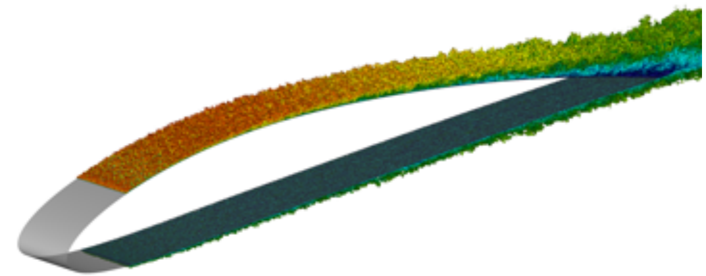
Y – Momentum:
$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho uv)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial(\rho vw)}{\partial z} = -\frac{\partial p}{\partial y} + \frac{1}{Re_r}\left[\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z}\right]$$

Z – Momentum
$$\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho uw)}{\partial x} + \frac{\partial(\rho vw)}{\partial y} + \frac{\partial(\rho w^2)}{\partial z} = -\frac{\partial p}{\partial z} + \frac{1}{Re_r}\left[\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z}\right]$$

Energy:
$$\frac{\partial(E_T)}{\partial t} + \frac{\partial(uE_T)}{\partial x} + \frac{\partial(vE_T)}{\partial y} + \frac{\partial(wE_T)}{\partial z} = -\frac{\partial(up)}{\partial x} - \frac{\partial(vp)}{\partial y} - \frac{\partial(wp)}{\partial z} - \frac{1}{Re_r Pr_r}\left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right]$$
$$+ \frac{1}{Re_r}\left[\frac{\partial}{\partial x}(u\tau_{xx} + v\tau_{xy} + w\tau_{xz}) + \frac{\partial}{\partial y}(u\tau_{xy} + v\tau_{yy} + w\tau_{yz}) + \frac{\partial}{\partial z}(u\tau_{xz} + v\tau_{yz} + w\tau_{zz})\right]$$

- Solution for one particular design

$$U = U(D(\boldsymbol{p}))$$

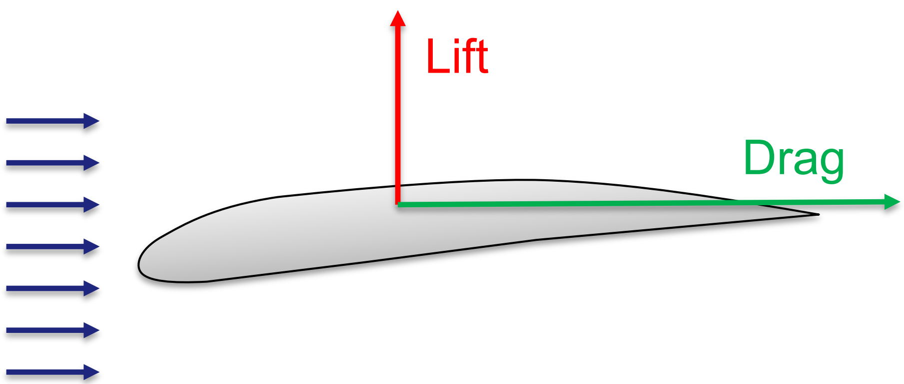


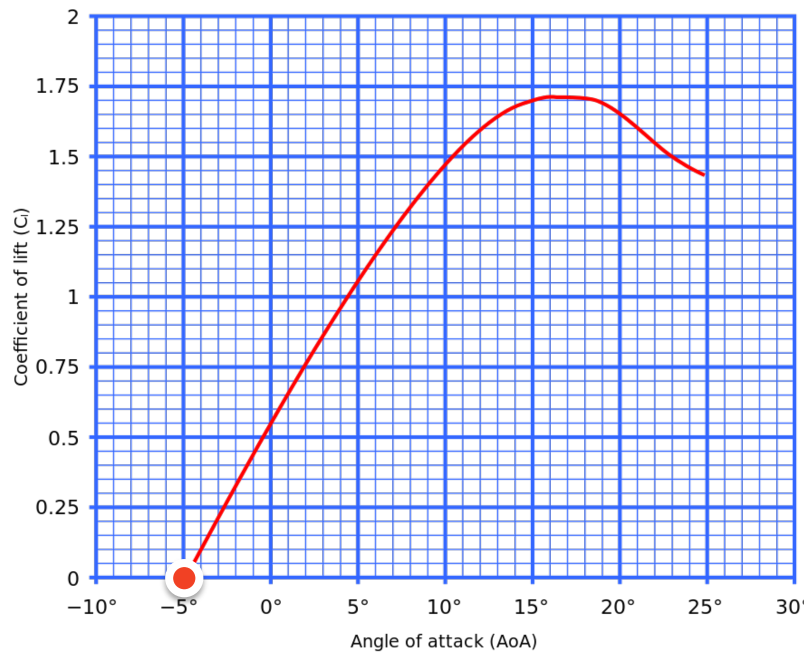
Linné FLOW Centre and SeRC, KTH, Sweden

3. Analysis

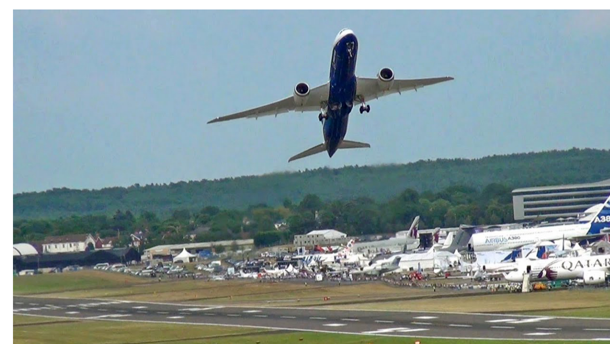
- Cost functional

$$\mathcal{C}(U;D)$$





Operation conditions

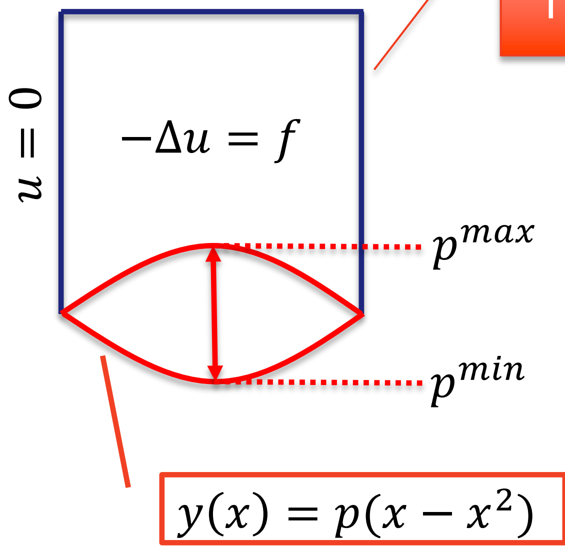


Abstract design optimization

- **Problem**: Find a set of admissible design parameters $\boldsymbol{p}$ such that solution $U(D(\boldsymbol{p}))$ to the mathematical model $\mathcal{M}(U, D(\boldsymbol{p}))$ computed on the design $D(\boldsymbol{p})$ optimizes the cost functional $\mathcal{C}(U, D(\boldsymbol{p}))$ for fixed operation condition

Academic model problem

1. Design



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

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

Quantum acceleration

- Best classical solution algorithm

  $\mathcal{O}(N s \kappa \log(1/\epsilon))$

- Quantum Linear Solver Algorithm

  - HHL: $\mathcal{O}(\log(N) s^2 \kappa^2 / \epsilon)$

  - Ambainis: $\mathcal{O}(\log(N) s^2 \kappa / \epsilon)$

Quantum acceleration

- Best classical solution algorithm

  $\mathcal{O}(N s \kappa \log(1/\epsilon))$

- Quantum Linear Solver Algorithm
  - HHL: $\mathcal{O}(\log(N) s^2 \kappa^2/\epsilon)$
  - Ambainis: $\mathcal{O}(\log(N) s^2 \kappa/\epsilon)$

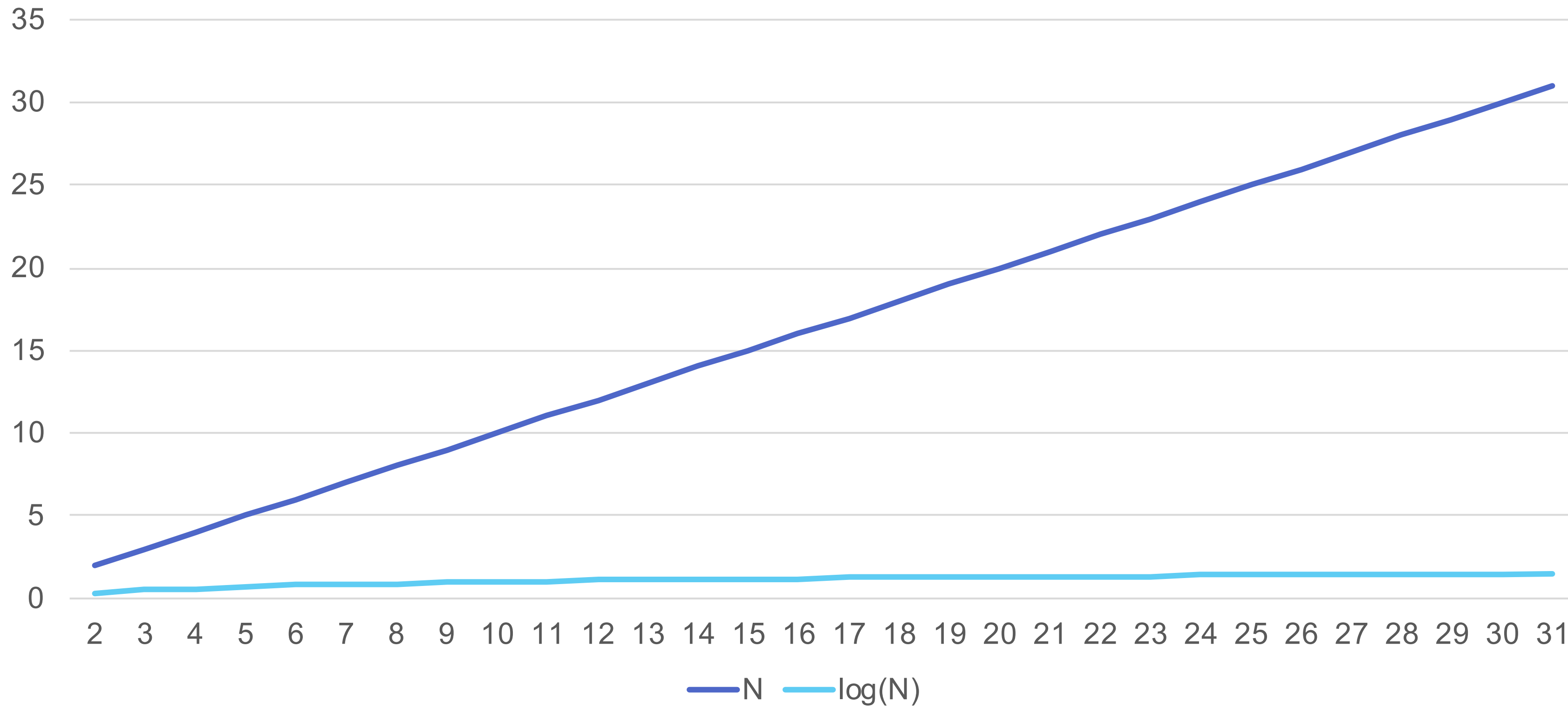
- Quadratic form optimizer

  $\mathcal{O}((\#\text{design parameters})^2)$

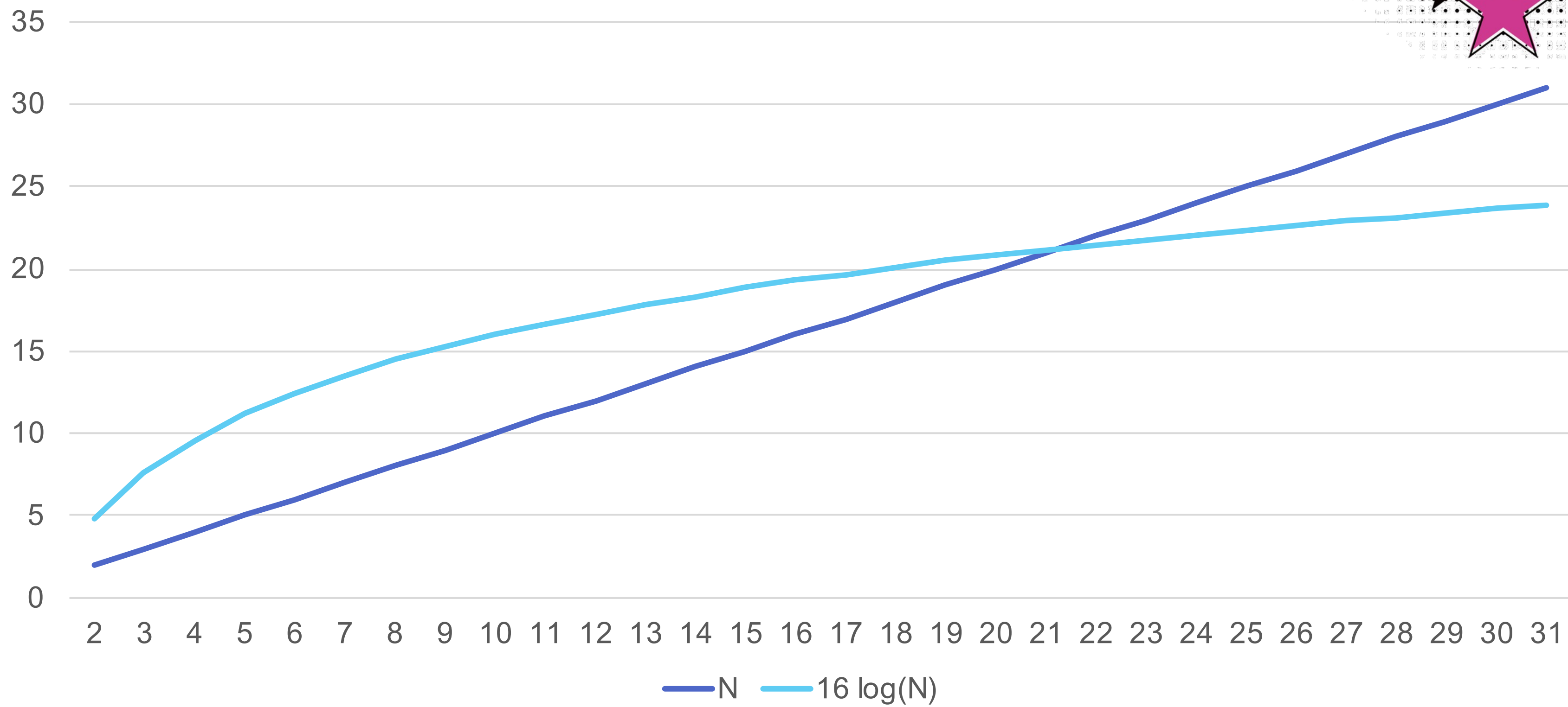
- Jordan's QOPT

  $\mathcal{O}((\#\text{design parameters})^1)$

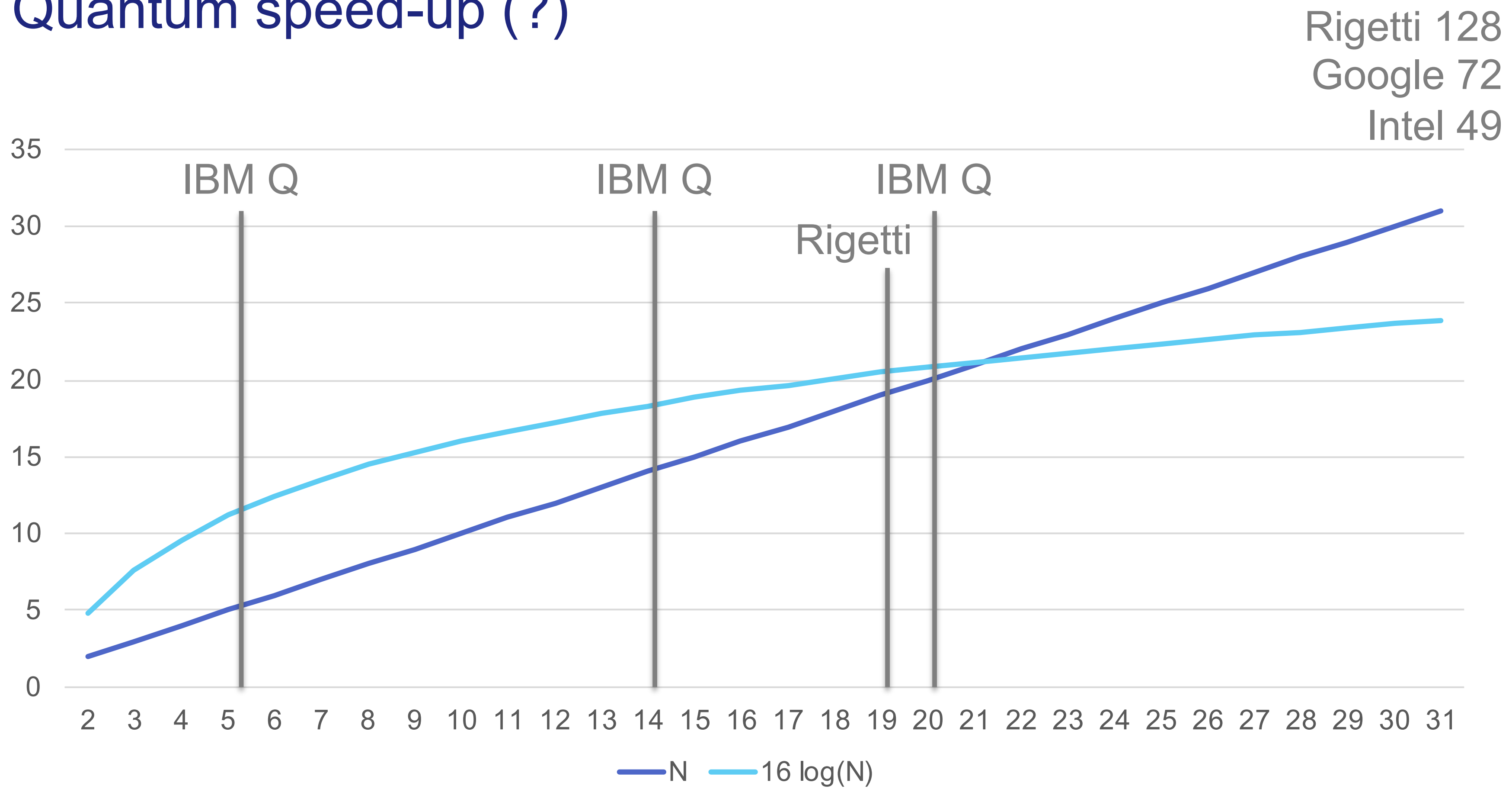
Quantum speed-up



Quantum speed-up (?)



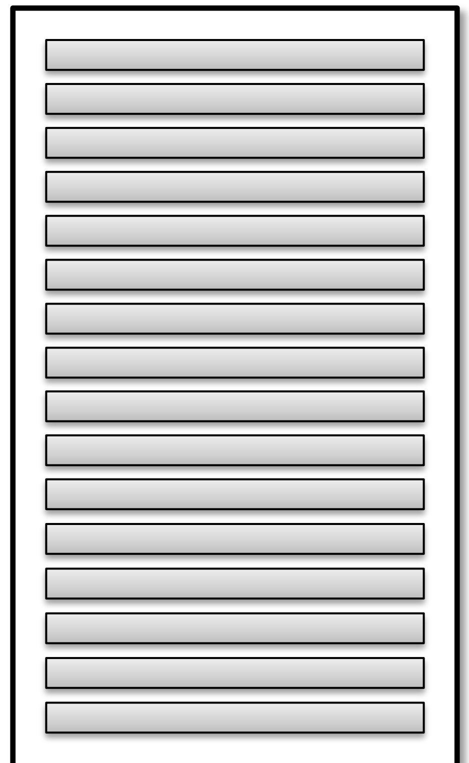
Quantum speed-up (?)



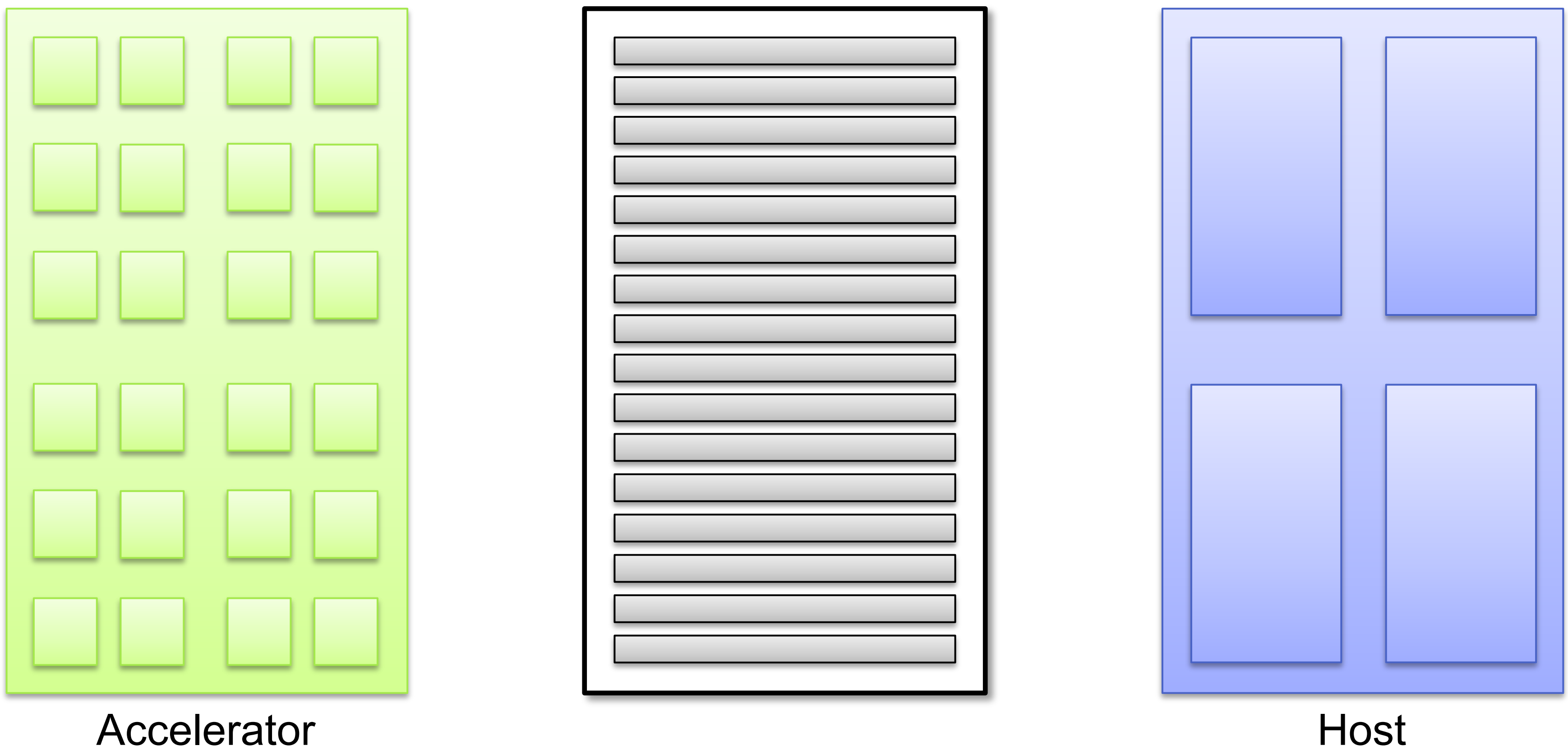
Practical aspects of quantum computing

SDKS AND GOOD PRACTICES

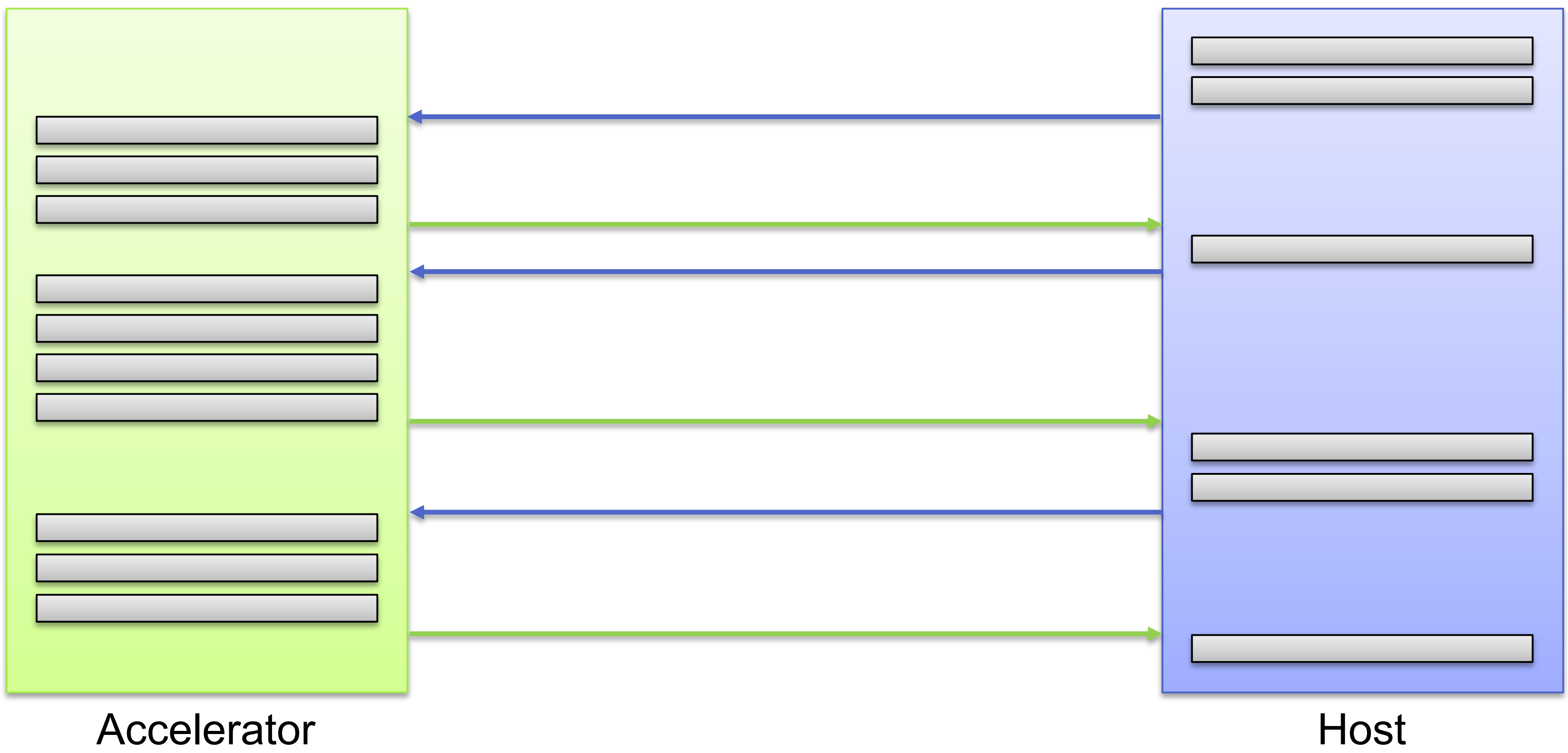
How accelerated computing works



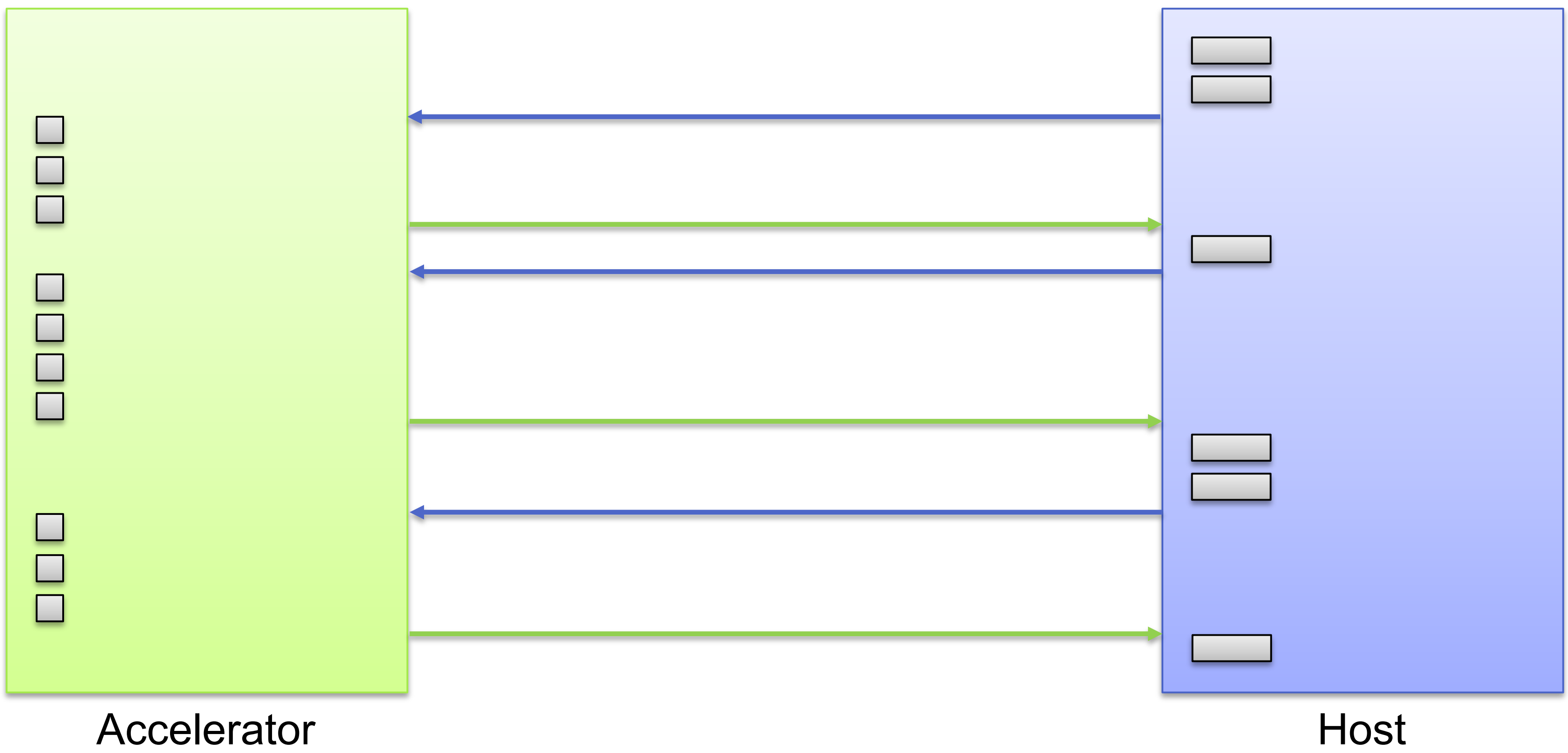
How accelerated computing works



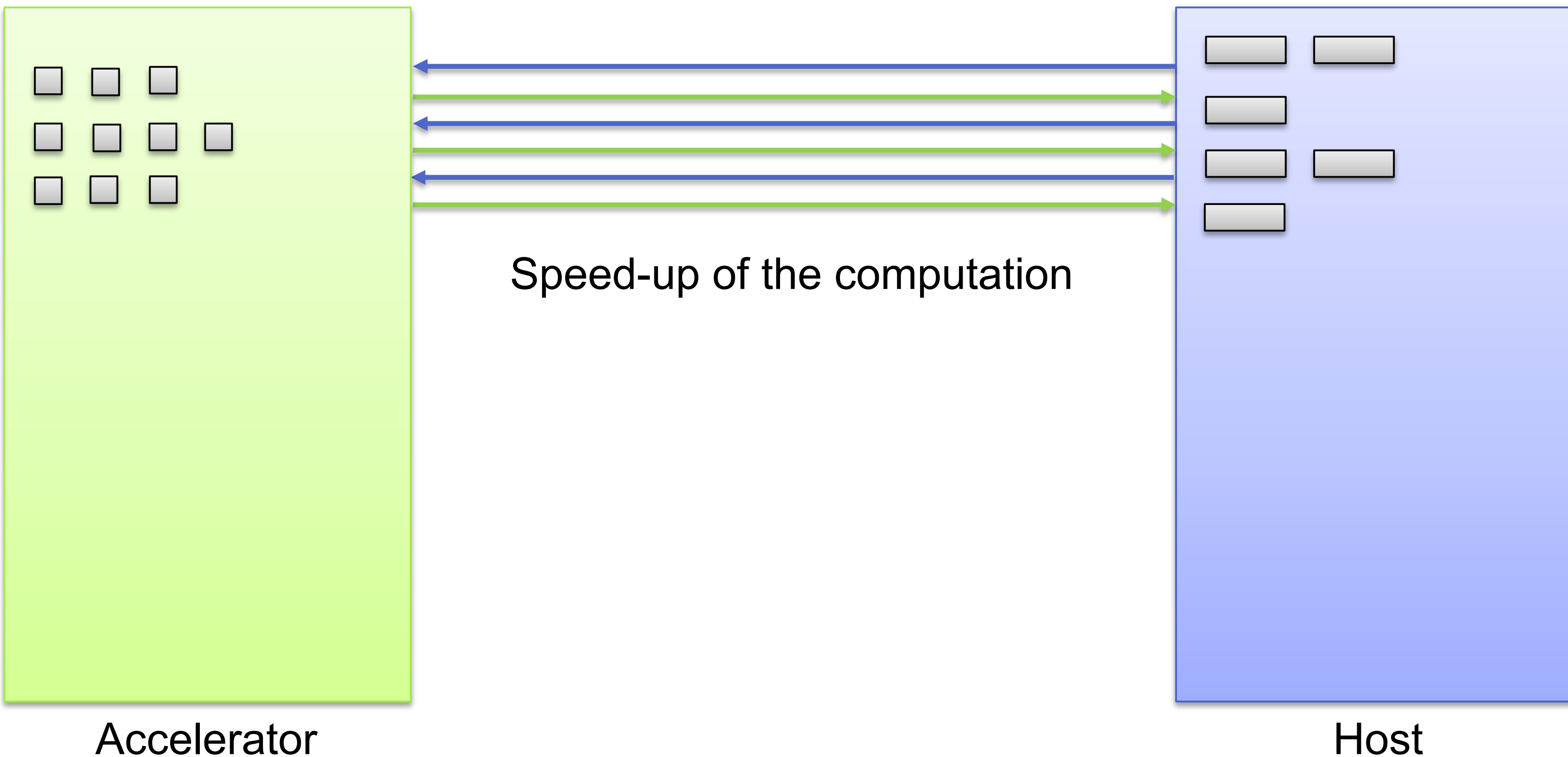
How accelerated computing works



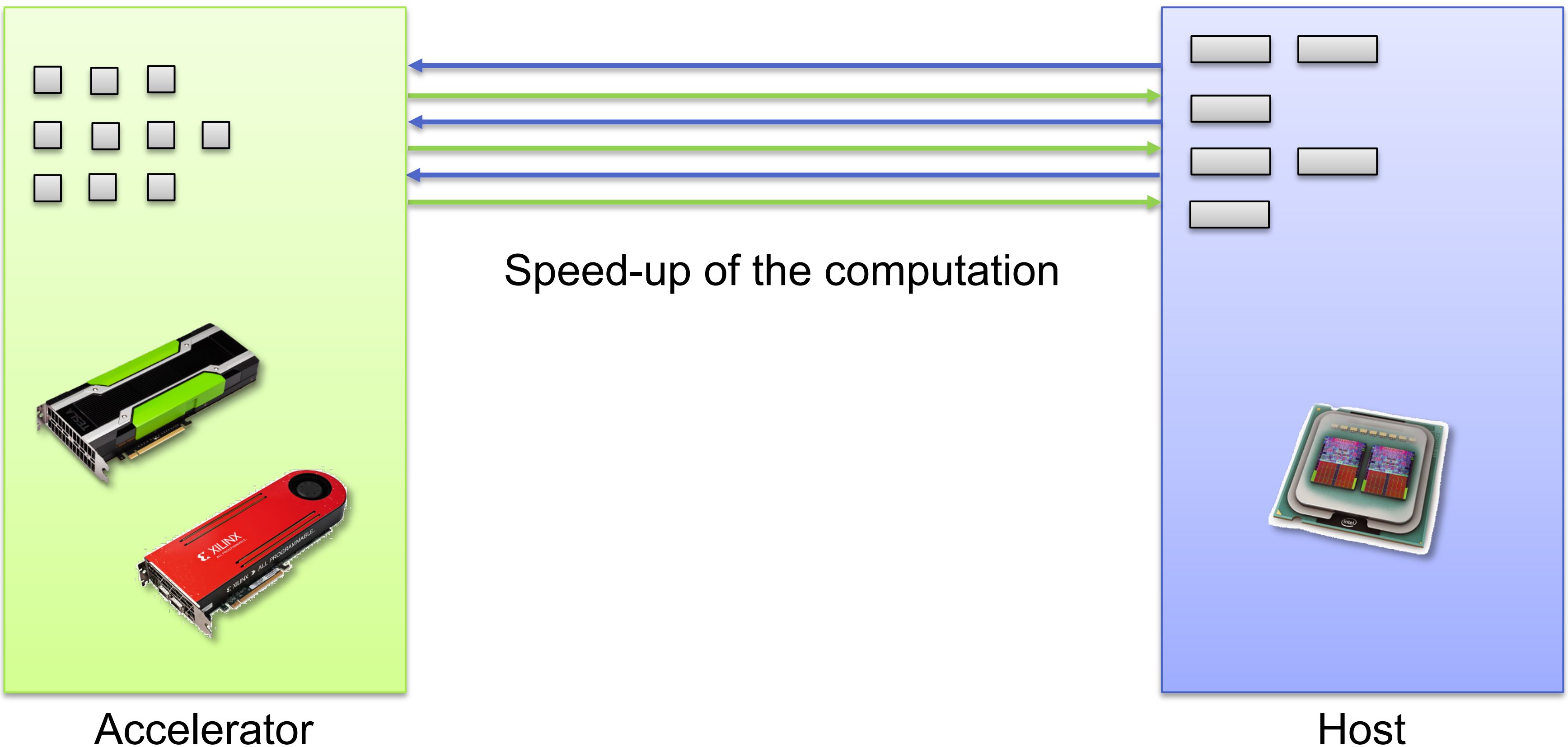
How accelerated computing works



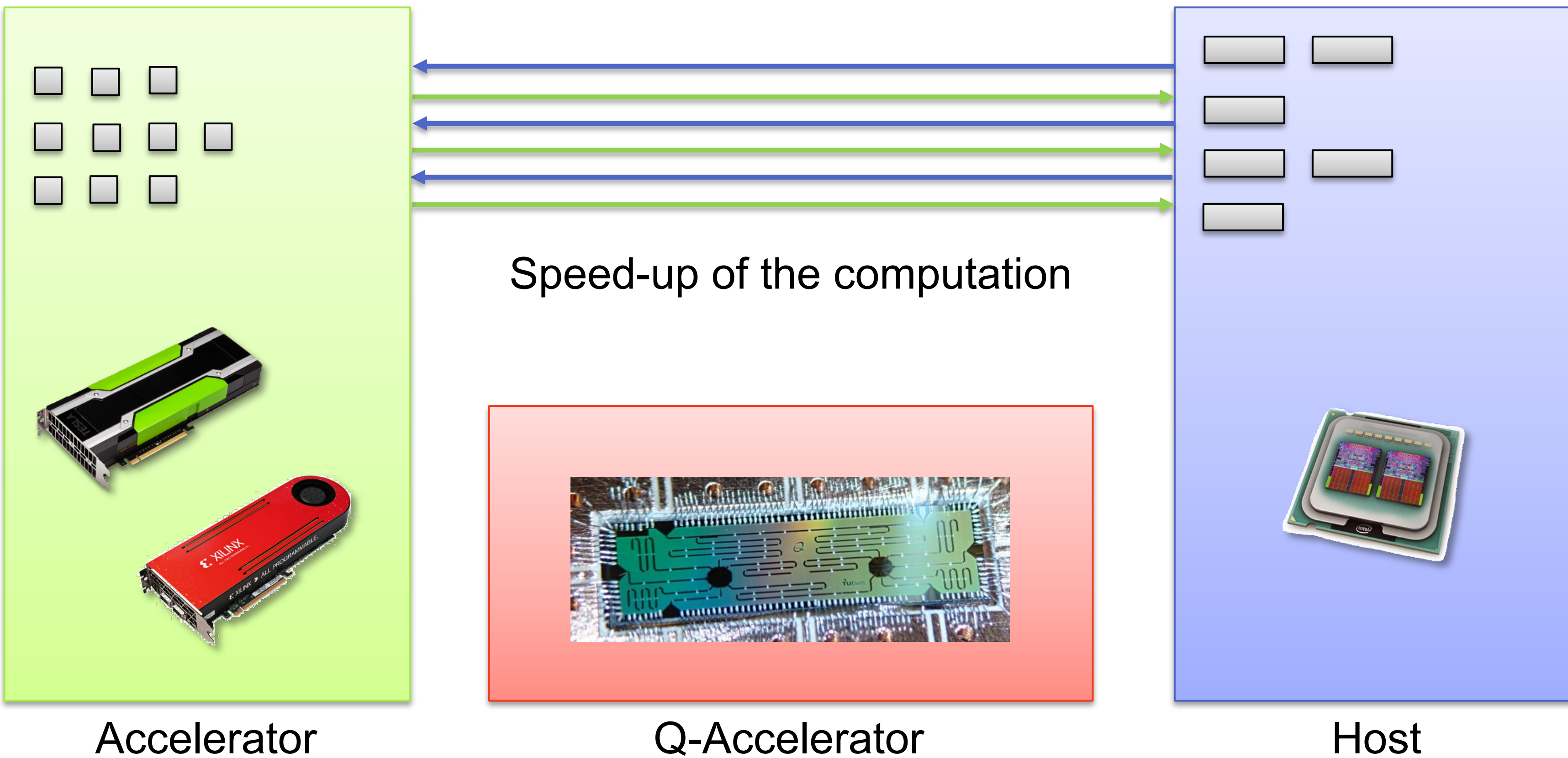
How accelerated computing works



How accelerated computing works



How accelerated computing works



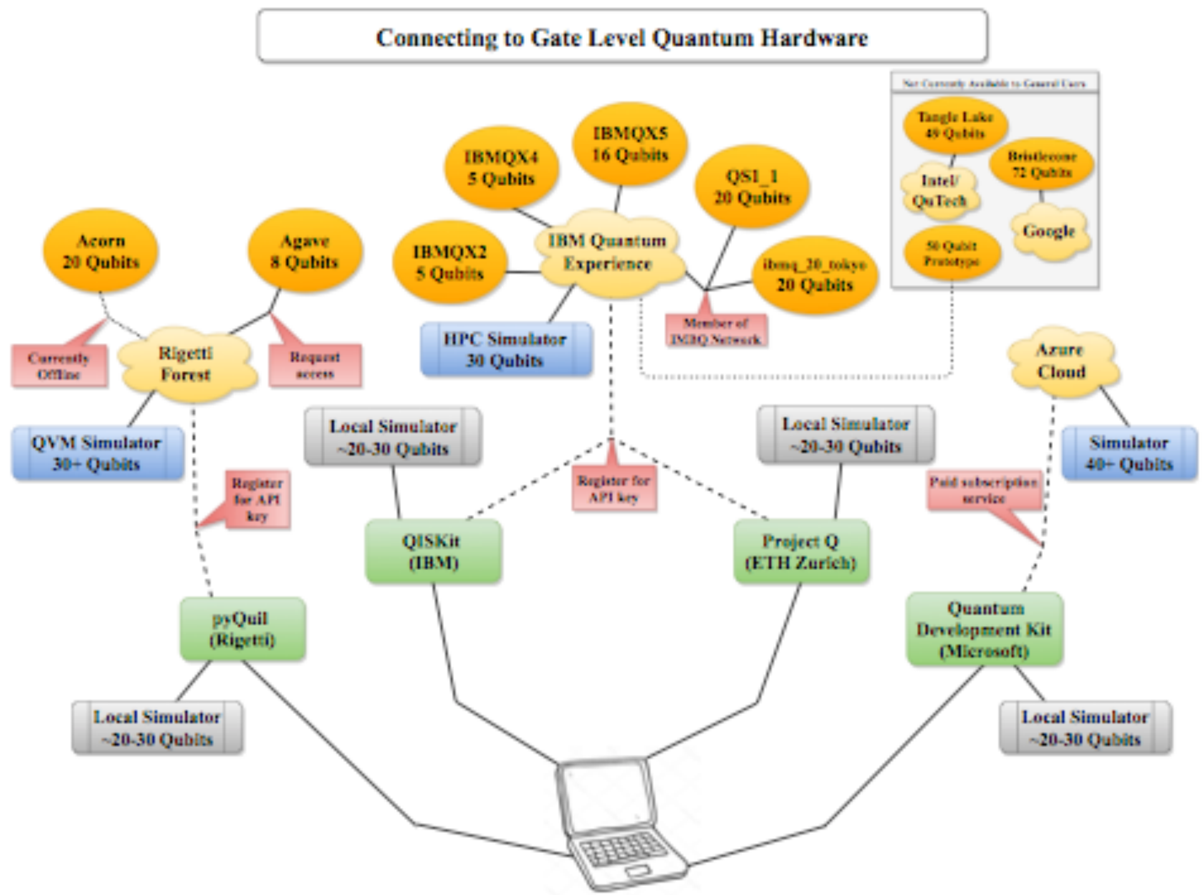
It feels like GPU-computing in the early 2000

- Quantum languages
  - AQASM: Atos QML
  - cQASM: QuTech QX, TNO QI
  - OpenQASM: IBM, Google
  - Quil: Rigetti
  - …

- Quantum SDKs
  - pyAqasm
  - pyQuil
  - Circ
  - OpenQL/QX
  - ProjectQ
  - QisKit
  - Quantum Development Kit
  - Quirk
  - …

It feels like GPU-computing in the early 2000

Algorithm	pyQuil	Qiskit	ProjectQ	QDK
Random Bit Generator	✓(T)	✓(T)	✓(T)	✓(T)
Teleportation	✓(T)	✓(T)	✓(T)	✓(T)
Swap Test	✓(T)			
Deutsch-Jozsa	✓(T)	✓(T)		✓(T)
Grover's Algorithm	✓(T)	✓(T)	✓(T)	✓(B)
Quantum Fourier Transform	✓(T)	✓(T)	✓(B)	✓(B)
Shor's Algorithm			✓(T)	✓(D)
Bernstein Vazirani	✓(T)	✓(T)		✓(T)
Phase Estimation	✓(T)	✓(T)		✓(B)
Optimization/ QAOA	✓(T)	✓(T)		
Simon's Algorithm	✓(T)	✓(T)		
Variational Quantum Eigensolver	✓(T)	✓(T)	✓(P)	
Amplitude Amplification	✓(T)			✓(B)
Quantum Walks		✓(T)		
Ising Solver	✓(T)			✓(T)
Quantum Gradient Descent	✓(T)			
Five Qubit Code				✓(B)
Repetition Code		✓(T)		
Steane Code				✓(B)
Draper Adder			✓(T)	✓(D)
Beauregard Adder			✓(T)	✓(D)
Arithmetic			✓(B)	✓(D)
Fermion Transforms	✓(T)	✓(T)	✓(P)	
Trotter Simulation				✓(D)
Electronic Structure (FCI, MP2, HF, etc.)			✓(P)	
Process Tomography	✓(T)	✓(T)		✓(D)
Vaidman Detection Test		✓(T)		



LaRose: Overview and Comparison of Gate Level Quantum Software Platforms, ArXiv, 2019

|LIB⟩: Kwantum expression template LIBrary

- Header-only C++14 library
- Open-source release by summer
- Auto-generation of quantum code from C++ expression templates
- Bi-directional communication between host and quantum device
- Made for quantum-accelerated *scientific* computing

|LIB⟩: Kwantum expression template LIBrary

```
auto expr = measure(h(x(h(x(init())))));
```

```
Qdata<1, OpenQASMv2> backend;
json result = expr(backend).execute();
```

```
QInt<3> a(1);
QInt<3> b(2);
a += b;
```

Conclusion

- Quantum computers have huge potential as special-purpose accelerators to speed-up the solution of (mathematical) problems ‘exponentially’
- Convergence towards common quantum programming language and development toolchain needed to make end-users interested (if at all!)
- To fully exploit the power of quantum computers don’t mimic classical algorithms but redesign quantum algorithms from scratch based on quantum-mechanical principles like superposition and entanglement

Thank you very much!