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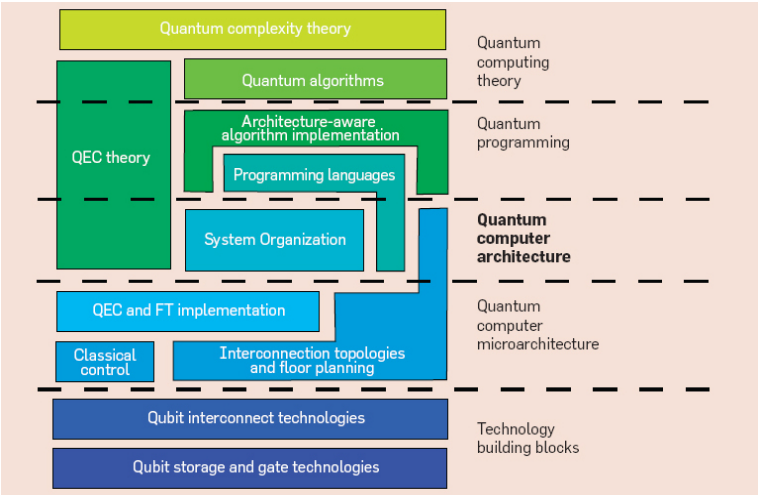
Formal Methods for Quantum Programs

Martin Avanzini **Georg Moser** Romain Péchoux Simon Perdrix
Vladimir Zamdzhiev

https://tcs-informatik.uibk.ac.at

A Bit of Context



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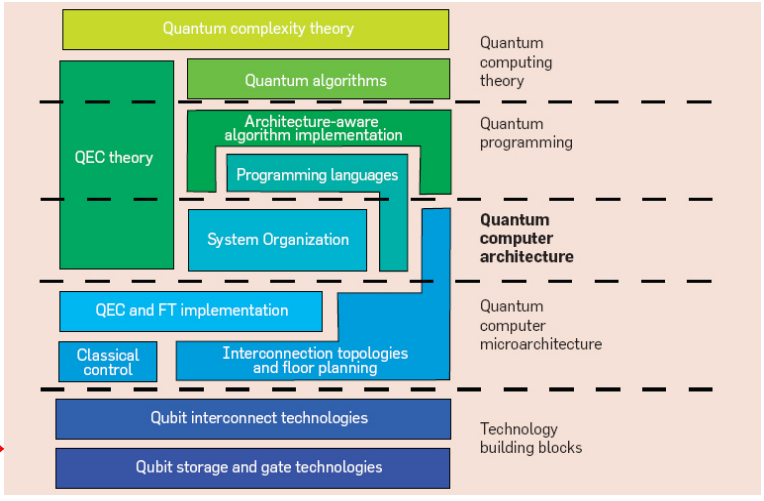

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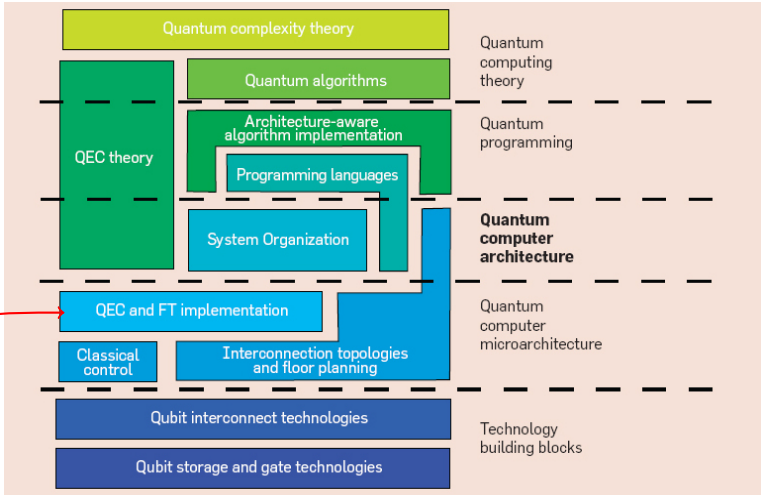
A Bit of Context



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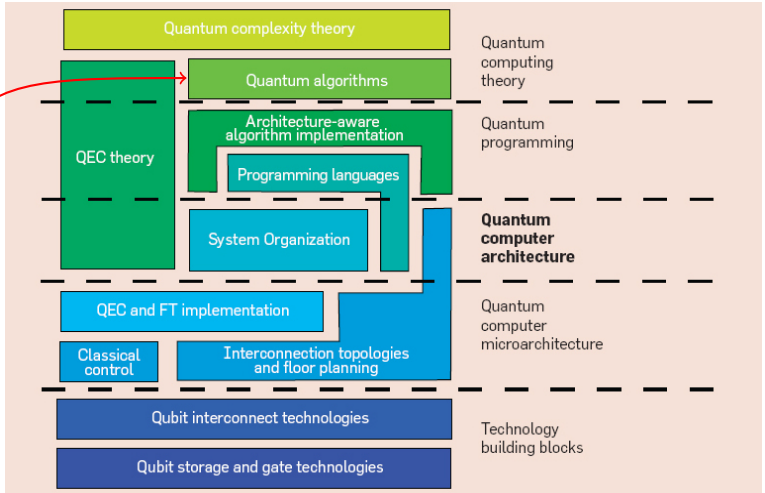

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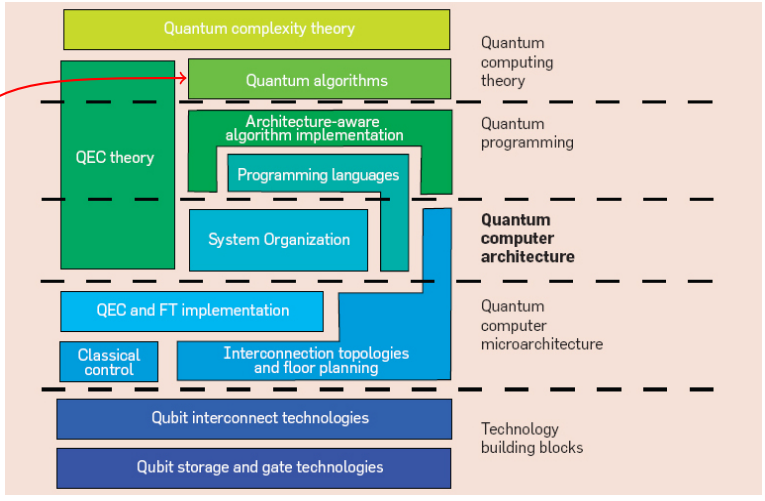

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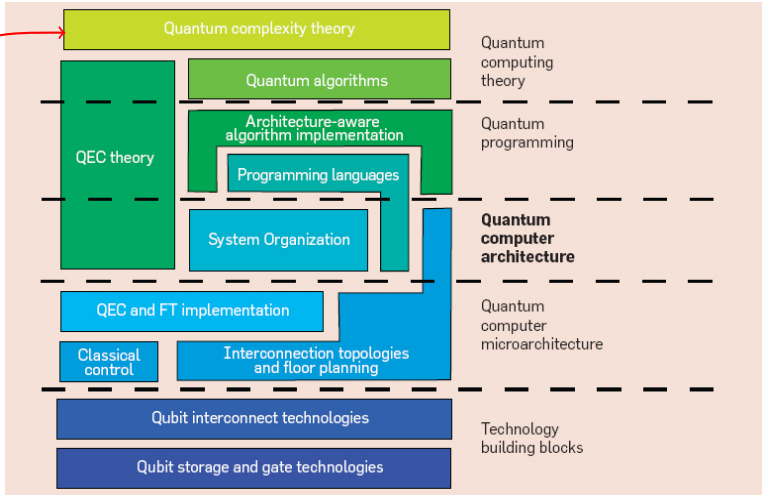

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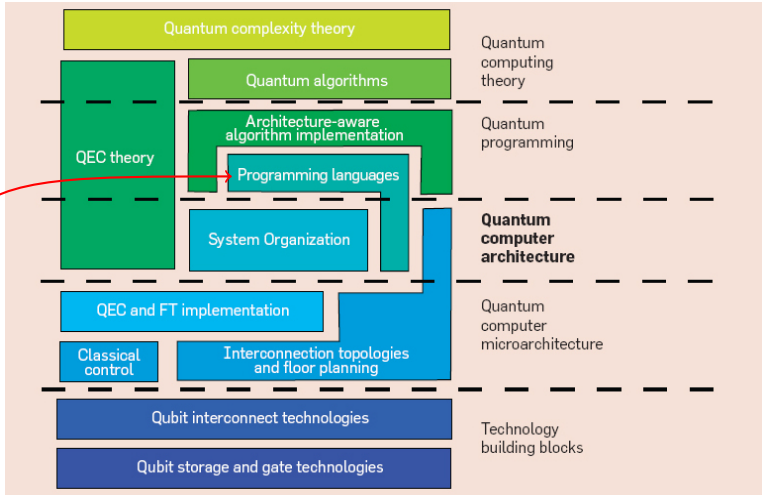

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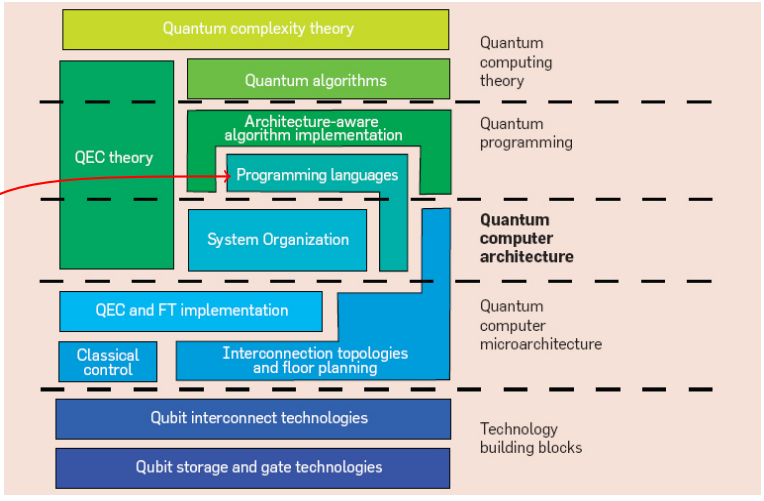

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Motivation to Study Quantum Computation

Viewpoint of Computer Science

1. quantum effects allows us to break the “strong” form of the Church-Turing thesis—any reasonable model of computation is efficiently computable by a Turing machine

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5. similarly, as quantum computers become the new normal, a theory of quantum programming languages is crucially needed

- **Quantum Programming Languages**
- **Program and Resource Analysis**
- **Expected Cost Analysis for Quantum Programs**

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Quantum Programming Languages

Requirements for Quantum Programming Languages

Allocation and Measurement

- allocate and measure quantum registers
- apply unitary operations

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Reasoning about Subroutines

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Building Quantum Oracles

- build quantum oracles from classical functions

Quantum Data Types

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- (quantum) data types allow for static type checking thus providing compile-time guarantees

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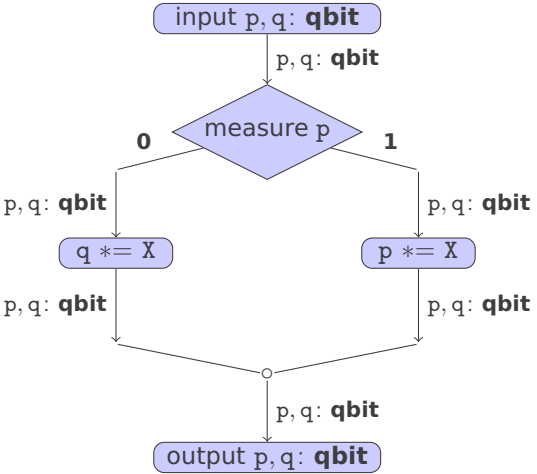
Resource Sensitivity and Resource Estimation

- estimation of resource requirements (eg. number of elementary gates, expected runtime)
- transparancies of quantum error correction

Selinger's Quantum Programming Language

Quantum Flow Language



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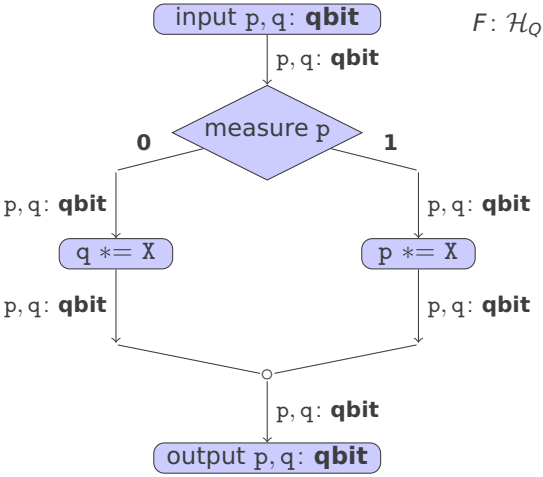
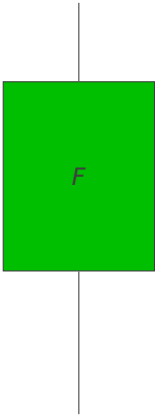


$F\colon \mathcal{H}_Q \xrightarrow{?} \mathcal{H}_Q$



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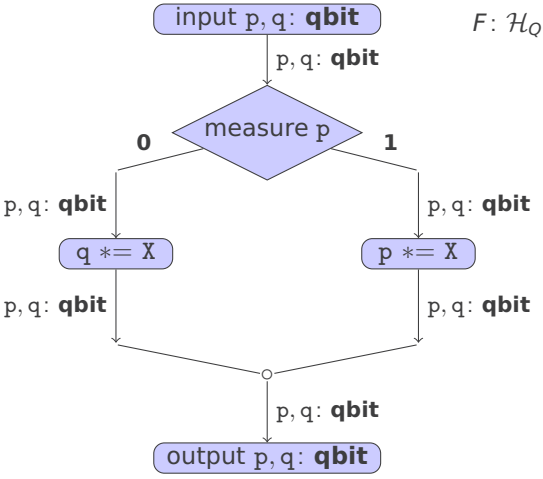

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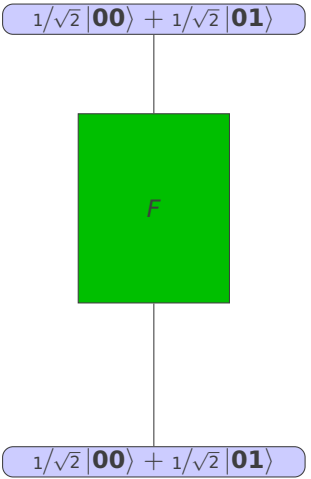

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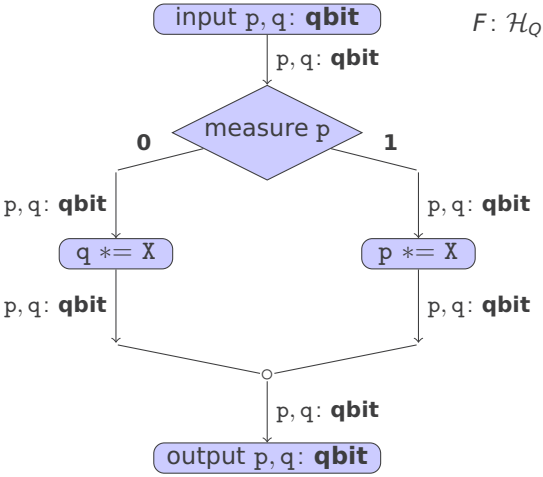

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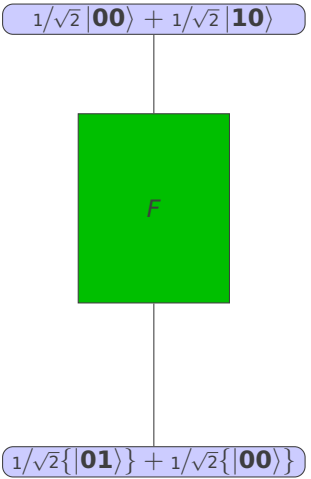

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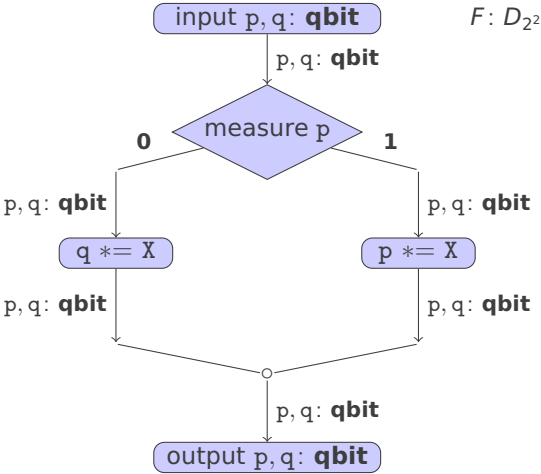
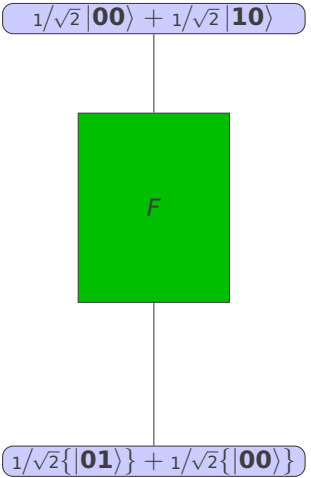
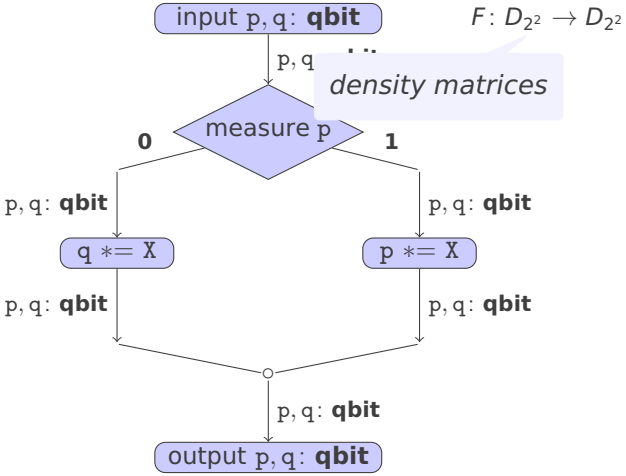


$F : D_{2^2} \to D_{2^2}$



Selinger's Quantum Programming Language

Quantum Flow Language



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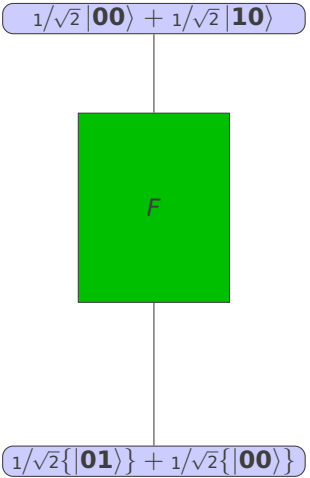
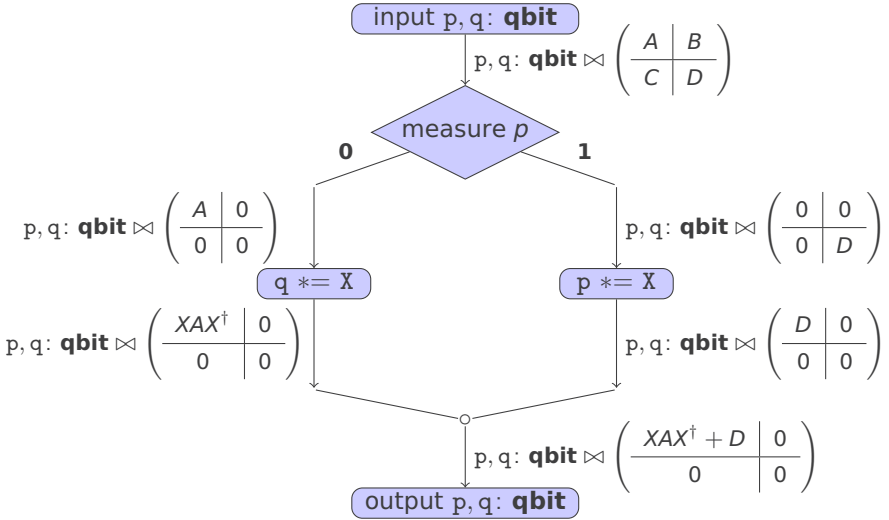
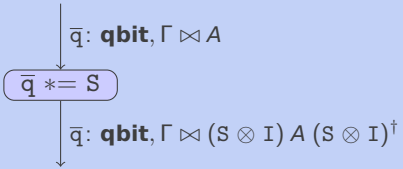


Quantum Flows Language (cont'd)



Focus on Unitary Transformation, Merge and Measurement

Unitary Transformation



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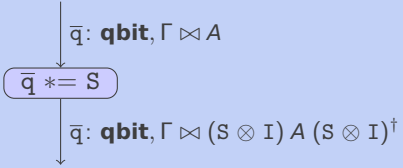

Example (Elementary Gates)

$$X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad H := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad T := \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}$$

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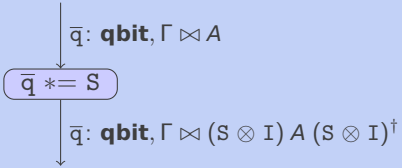
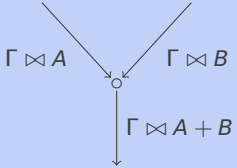
Unitary Transformation



Merge



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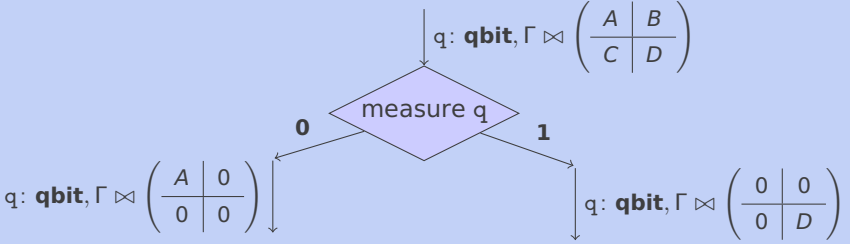
Measurement



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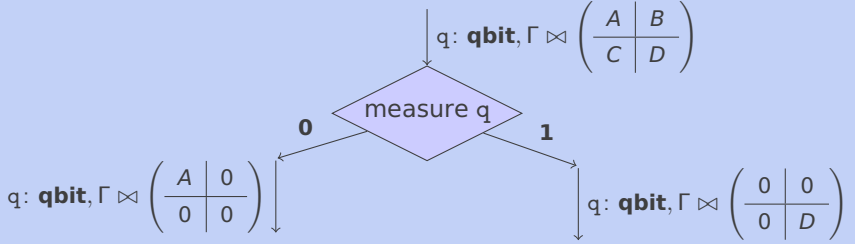
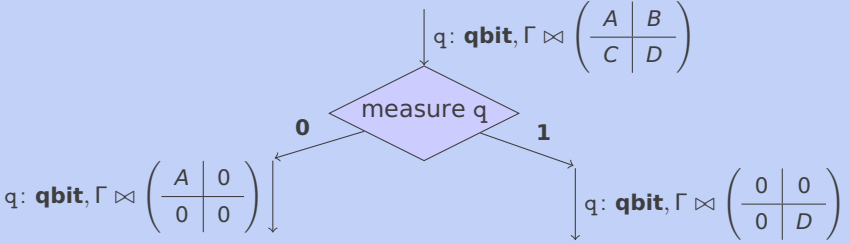


- let $|\varphi\rangle$ be a pure state, s.t.

$$|\varphi\rangle = \begin{pmatrix} v \\ \hline w \end{pmatrix} \qquad |\varphi\rangle\langle\varphi| = \left(\begin{array}{c|c} vv^\dagger & vw^\dagger \\ \hline wv^\dagger & ww^\dagger \end{array}\right)$$

Measurement



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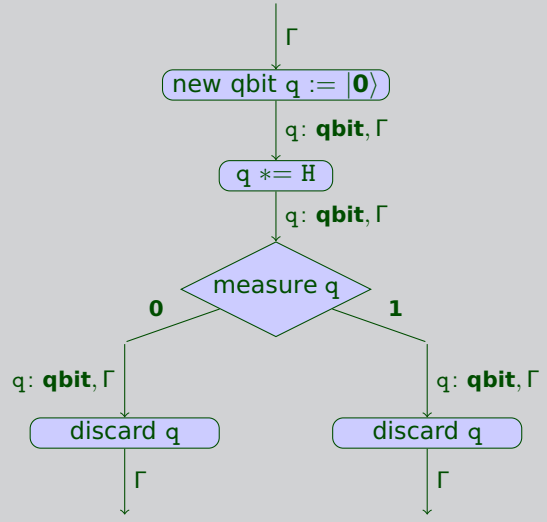
- measuring the first qubit of $|\varphi\rangle$ in the computational basis, yields

$$\|v\|^2 : \left(\begin{array}{c|c} vv^\dagger & 0 \\ \hline 0 & 0 \end{array}\right) \qquad \|w\|^2 : \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & ww^\dagger \end{array}\right)$$

Example (Coin Toss)



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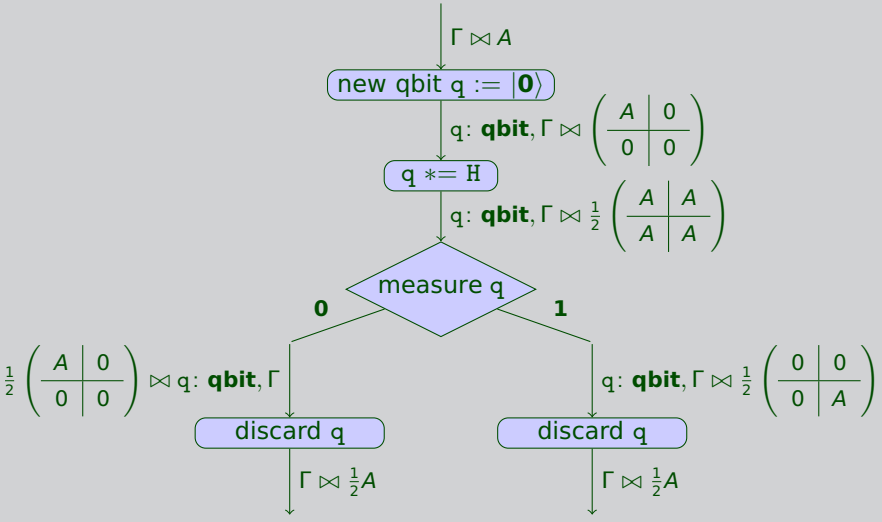

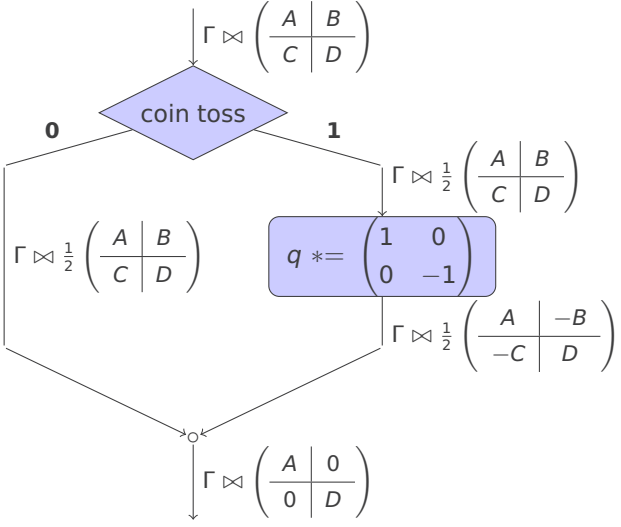
$\Gamma \bowtie \left(\begin{array}{c|c} A & B \\ \hline C & D \end{array}\right)$
coin toss
0
1
$\Gamma \bowtie \frac{1}{2} \left(\begin{array}{c|c} A & B \\ \hline C & D \end{array}\right)$
$q \mathrel{*}= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
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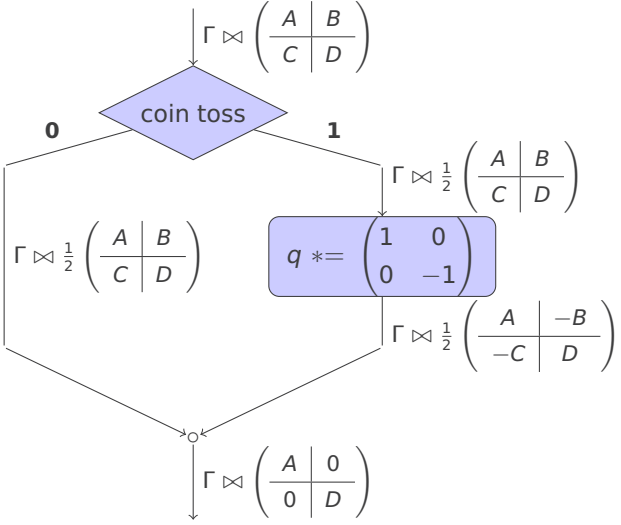
Semantical Program Equivalence



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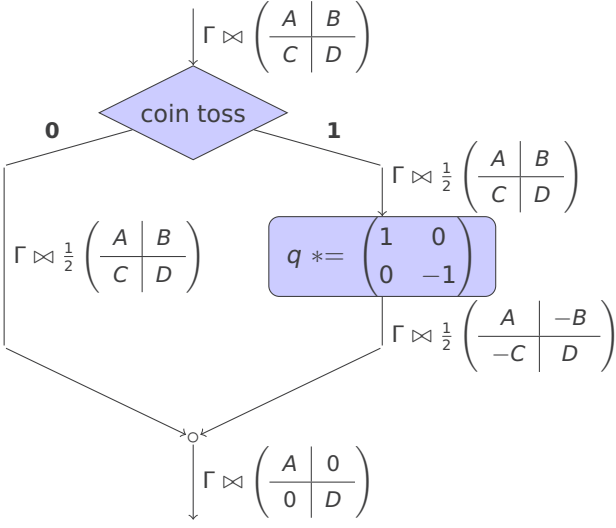
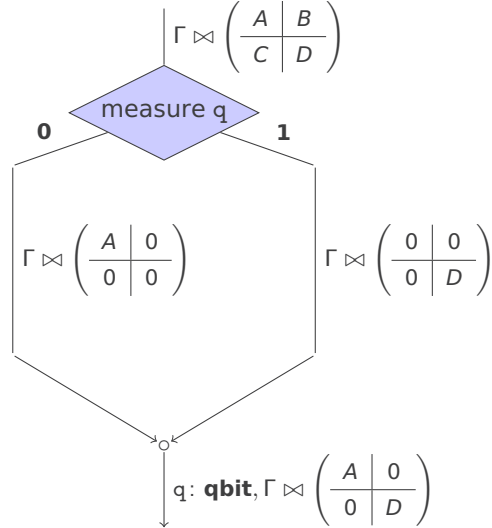
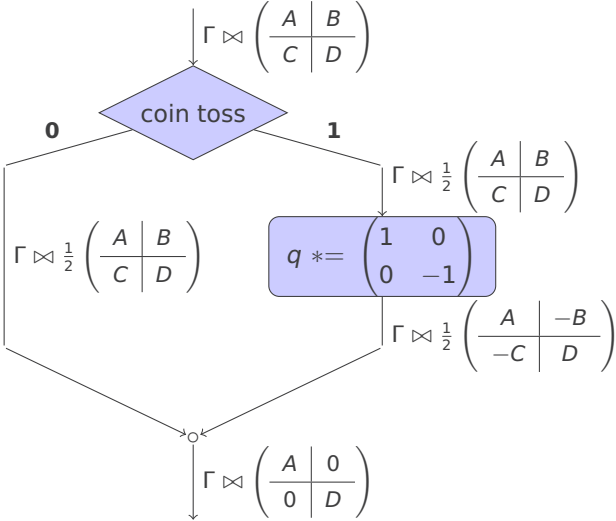
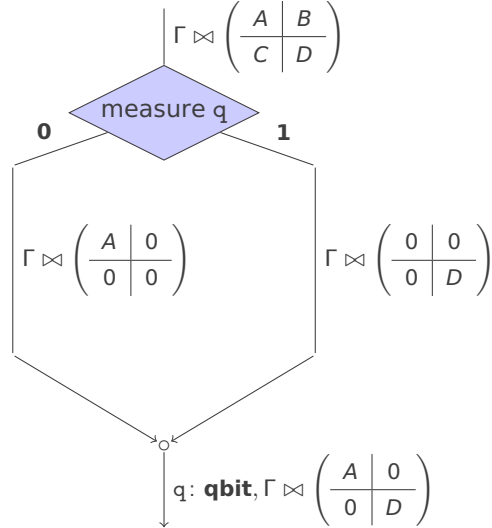




Semantical Program Equivalence: Program Optimisation





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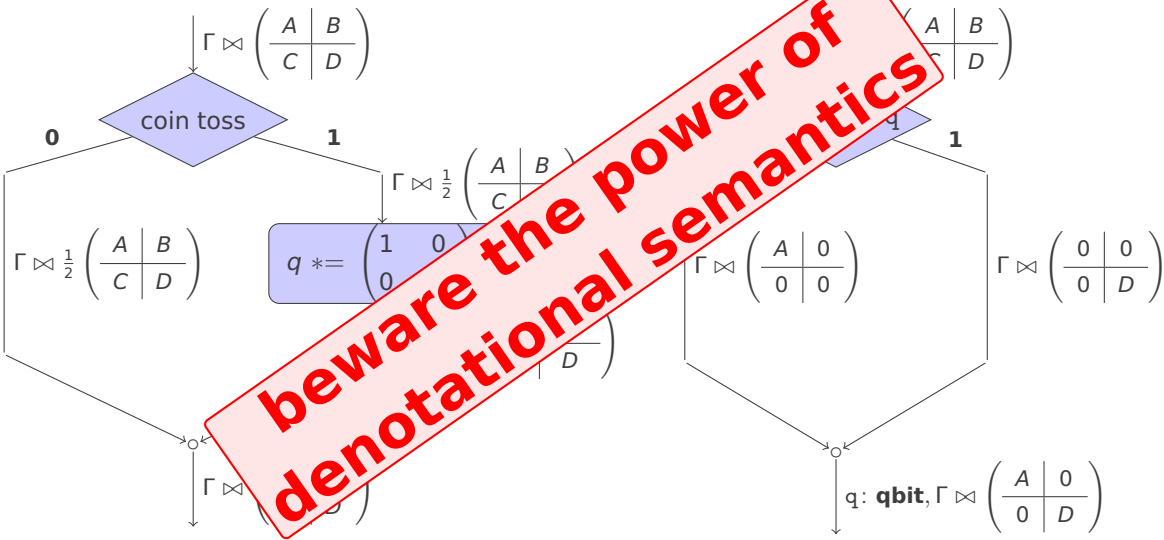

beware the power of denotational semantics

The Language QPL

QPL Terms

$$
\begin{aligned}
\texttt{stm}, \texttt{stm}_1, \texttt{stm}_2 \quad ::= \quad & \texttt{new bit b} := \mathbf{0} \mid \texttt{new qbit b} := |\mathbf{0}\rangle \mid \texttt{discard x} \\
& \mid \texttt{b} := \mathbf{0} \mid \texttt{b} := \mathbf{1} \mid \texttt{q}_1, \ldots, \texttt{q}_n \mathrel{*}= \texttt{S} \\
& \mid \texttt{skip} \mid \texttt{stm}_1 ; \texttt{stm}_2 \mid \\
& \mid \texttt{if}(\texttt{b}) \texttt{ then } \texttt{stm}_1 \texttt{ else } \texttt{stm}_2 \mid \texttt{measure q then } \texttt{stm}_1 \texttt{ else } \texttt{stm}_2 \\
& \mid \texttt{while b stm} \\
& \mid \texttt{proc } X \colon \Gamma \to \Gamma' \, \{\texttt{stm}_1\} \texttt{ in } \texttt{stm}_2 \mid \texttt{y}_1, \ldots, \texttt{y}_m := X(\texttt{x}_1, \ldots, \texttt{x}_n)
\end{aligned}
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\end{aligned}
$$

Comments

- $\texttt{proc } X\colon \Gamma \to \Gamma' \{\texttt{stm}_1\} \texttt{ in stm}_2$ defines a procedure with body $\texttt{stm}_1$ and scope $\texttt{stm}_2$
- $\texttt{y}_1, \ldots, \texttt{y}_m {=} X(\texttt{x}_1, \ldots, \texttt{x}_n)$ denotes a procedure call

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\end{aligned}
$$

Comments

- $\texttt{proc } X\colon \Gamma \to \Gamma' \{\texttt{stm}_1\} \texttt{ in stm}_2$ defines a procedure with body $\texttt{stm}_1$ and scope $\texttt{stm}_2$
- $\texttt{y}_1, \ldots, \texttt{y}_m {=} X(\texttt{x}_1, \ldots, \texttt{x}_n)$ denotes a procedure call

Summary on QPL

- each edge in the quantum flow chart has been given an annotation in the form of a density matrix
- the semantics of a QPL program is now given as a mapping of the input density matrix to the output density matrix
- in order to show well-definedness these mapping are couched as morphisms of a category based on superoperators
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Q#	✓	✓	✓	✓	×	×

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Program and Resource Analysis

Static Program Analysis

Definition (due to Z. Manna and A. Pnueli)

"The algorithmic discovery of properties of a program by inspection of the source text."

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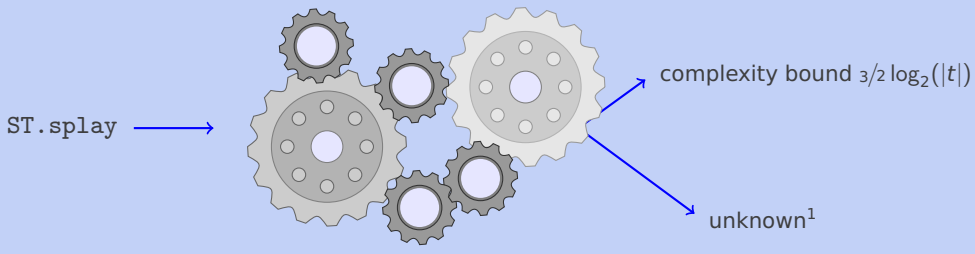

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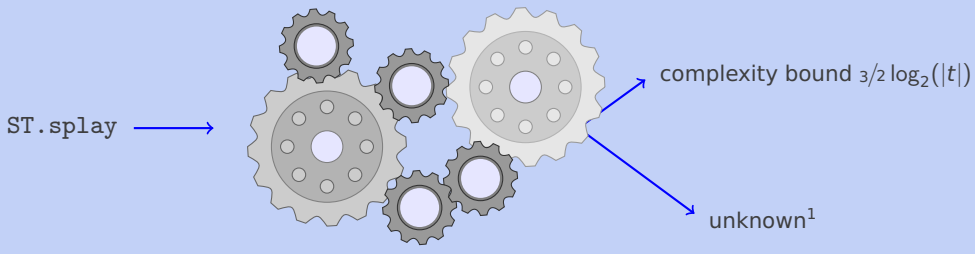

[1]The problem is (highly) undecidable, to be precise it is Σ_2^0-complete.

Zune Bug: December 31, 2008


```
year = ORIGINYEAR; /* = 1980 */
while (days > 365) {
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SOLVED!

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Quantum Bugs

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Quantum Bugs

- empirical study of bugs in a broad range of quantum computing platforms (eg. IBM's Qiskit, Google's Circ, Mircosoft's Q#)
- research methodology: search for commit message like "fix" together with evidence of a commit that patched the problem
- 223 bugs found, among them (almost) 40% quantum-specific

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- research methodology: search for commit message like "fix" together with evidence of a commit that patched the problem
- 223 bugs found, among them (almost) 40% quantum-specific
- bugs occur everywhere, quantum-specific ones parts that represent, compile or optimise quantum code
- classical bugs occur in seemingly easy adminstrative code, like infrastructural scripts
- study proposes a hierarchy of bug patterns: ten quantum-specific patterns

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Quantum-Specific Patterns

Incorrect Numerical Calculation

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return pauli_string_phasor.PauliStringPhasor(
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- testing doesn't help
- compile-time guarantees through better type systems or specification languages would

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```

not at all solved
formal methods required

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Expected Cost Analysis for Quantum Programs

Resource Analysis of Quantum Programs

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- the expected runtime
- the expected number of quantum gates
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Coin Tossing: Syntax by Example

$$
\begin{array}{l}
CT(\mathtt{q}) \triangleq\ \mathtt{x} = \mathtt{true};\\
\qquad\quad \mathtt{while(x)\{}\\
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\qquad\qquad \mathtt{x} = \mathtt{meas(q)};\\
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\qquad\qquad \}
\end{array}
\Bigg\}\mathtt{stm}_0
$$

- iterated coin toss, probability of termination after n steps depends on initial state $|\varphi\rangle$ of qubit q
- loop body $\mathtt{stm}_0$ consumes 1 resource
- overall probability of termination $= 1$

Coin Tossing: Syntax by Example

$$\mathtt{stm}, \mathtt{stm}_1, \mathtt{stm}_2 \quad ::= \quad \mathtt{skip} \mid \mathtt{x}^{\mathcal{K}} = \mathtt{e}^{\mathcal{K}} \mid \overline{\mathtt{q}} \mathrel{*}= \mathtt{U} \mid \mathtt{x}^{\mathcal{B}} = \mathtt{meas(q)} \mid \mathtt{consume(a)} \mid \mathtt{stm}_1; \mathtt{stm}_2 \mid \mathtt{if}\ (\mathtt{b})\ \{\mathtt{stm}_1\}\ \mathtt{else}\ \{\mathtt{stm}_2\} \mid \mathtt{while(b)}\ \{\mathtt{stm}\}$$

- a state σ is a pair $(s, |\varphi\rangle)$ consisting of a store s and a quantum state $|\varphi\rangle$
- a configuration μ is pair $(\mathtt{stm}, \sigma)$

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Coin Tossing: Expected Cost Analysis

Manual Analysis

- let $(s, |\varphi\rangle)$ be a state, s.t.
  - $s(x) = \texttt{true}$
  - $|\varphi\rangle = \alpha\,|\mathbf{0}\rangle + \beta\,|\mathbf{1}\rangle$

$$\mathrm{ecost}_{CT(\mathsf{q})}(s, \begin{pmatrix}\alpha\\ \beta\end{pmatrix}) = \sup_{n\in\mathbb{N}} \left\{1 + p_1 \textstyle\sum_{i=0}^{n} \frac{1}{2^i}\right\} = 1 + |\alpha - \beta|^2$$

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requires

- formal operational semantics (roughly $[\![\mathtt{stm}]\!] \colon \mathtt{State} \to \mathcal{D}(\mathtt{State})$)
- semantics accounts for resource consumption
- but tedious, error-prone calculations!

Quantum Expected Cost Transformer

(generalisation of Hoare-style formal verification)

$$\mathtt{qect}\left[\cdot\right]\left\{\cdot\right\} : \mathtt{Program} \to (\mathtt{State} \to \mathbb{R}^{+\infty}) \to (\mathtt{State} \to \mathbb{R}^{+\infty})$$

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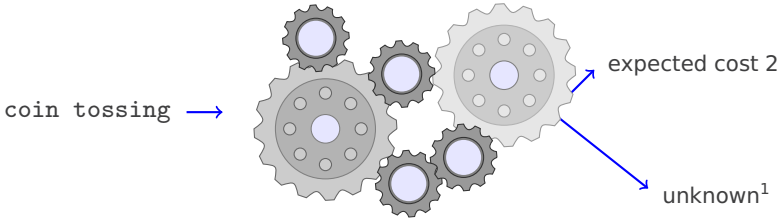
Theorem

The following identity hold, for all $\mathtt{stm} \in \mathtt{Statement}$ *and* $\sigma \in \mathtt{State}$

$$\mathtt{qect}\left[\mathtt{stm}\right]\left\{\underline{0}\right\}(\sigma) = \mathrm{ecost}_{\mathtt{stm}}(\sigma)$$

Illustrating Examples



`stm`	cost metric	expect cost
coin tossing	# of loops	2
repeat-until-success	# of T gates	$\frac{8}{3}$
entangled state preparation	# of attempts for k qubits	$148 \cdot (k+4)$
quantum walk on n-circle	# of loops	2 if started at position $\lvert\mathbf{1}\rangle$ 1 if started at position $\lvert\mathbf{0}\rangle$

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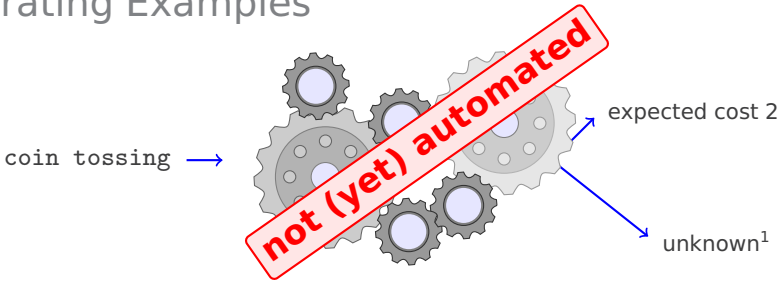

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$CT(\mathtt{q}) \triangleq$
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```
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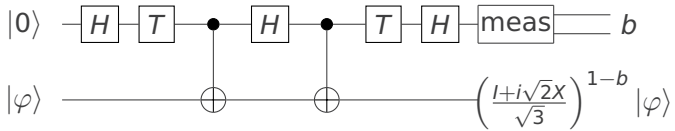

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Illustrating Examples

$CHAIN(k, q_0, \ldots, q_{k+3}) \triangleq$

```
  ...
  while(0 ≤ t ∧ t < k){
    CHAIN4(q_{t+1}, q_{t+2}, q_{t+3}, q_{t+4});
    FUSE(q_t, q_{t+1}, x);
    if(x){t = t + 4} else {t = t − 1};
    if(t = −1){t = 0; q_0 = |+⟩} else {skip}
  }
```

- prepare a graph state represented by a path on k qubits
- implemented with nested while loops

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$\Sigma_{i=0}^{n-1} |L\rangle\langle L| \otimes |i \ominus 1\rangle\langle i| + \Sigma_{i=0}^{n-1} |R\rangle\langle R| \otimes |i \oplus 1\rangle\langle i|$

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Comparison

	Allocation	Subroutines	Oracles	Data Types	Specification	Resources
qWhile	✓	×	×	(✓)	(✓)	✓

M. Avanzini, G. Moser, R. Péchoux, S. Perdrix, and V. Zamdzhiev.
Quantum expectation transformers for cost analysis. *CoRR*, abs/2201.09361, 2022.

Thank You For Your Attention!

Quantum Expectation Transformer

$\mathtt{stm}$	$\mathtt{qet}\left[\mathtt{stm}\right]\left\{f\right\}$
ϵ	f
$\mathtt{skip}$	f
$\mathtt{x} = \mathtt{e}$	$f[\mathtt{x} := \mathtt{e}]$
$\overline{\mathtt{q}} *= \mathtt{U}$	$f[\mathtt{U}_{\overline{\mathtt{q}}}]$
$\mathtt{x} = \mathtt{meas}(\mathtt{q})$	$p_0^{\mathtt{q}} f[\mathtt{x} := 0; \mathtt{M}_0^{\mathtt{q}}] + (1 - p_0^{\mathtt{q}}) f[\mathtt{x} := 1; \mathtt{M}_1^{\mathtt{q}}]$
$\mathtt{consume}(\mathtt{a})$	$\max(\llbracket \mathtt{a} \rrbracket, \underline{0}) + f$
$\mathtt{stm}_1; \mathtt{stm}_2$	$\mathtt{qet}\left[\mathtt{stm}_1\right]\left\{\mathtt{qet}\left[\mathtt{stm}_2\right]\left\{f\right\}\right\}$
$\mathtt{if}(\mathtt{b})\{\mathtt{stm}_1\}\ \mathtt{else}\ \{\mathtt{stm}_2\}$	$\mathtt{qet}\left[\mathtt{stm}_1\right]\left\{f\right\} +_{\llbracket \mathtt{b} \rrbracket} \mathtt{qet}\left[\mathtt{stm}_2\right]\left\{f\right\}$
$\mathtt{while}(\mathtt{b})\{\mathtt{stm}\}$	$\mathrm{lfp}\left(\lambda F.\mathtt{qet}\left[\mathtt{stm}\right]\left\{F\right\} +_{\llbracket \mathtt{b} \rrbracket} f\right)$

Coin Tossing: Formal Expected Cost Analysis

- we need to find an expectation g satisfying the following inequalities

$$[\![\neg \mathtt{x}]\!] \cdot \underline{0} \leqslant g$$
$$[\![\mathtt{x}]\!] \cdot \mathtt{qect}\Big[\mathtt{stm}_0\Big]\Big\{g\Big\} \leqslant g$$

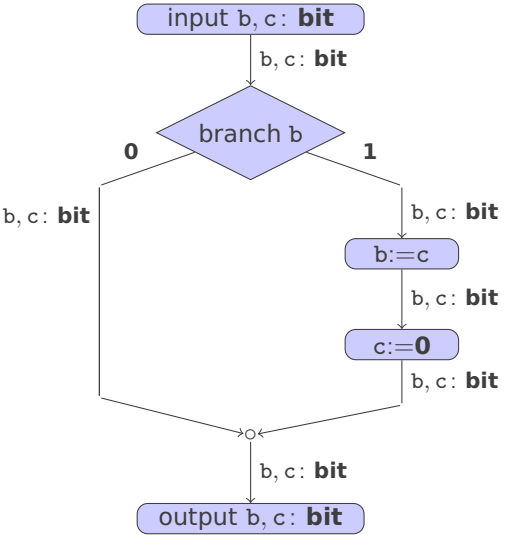
- we set

$$g(s, \begin{pmatrix} \alpha \\ \beta \end{pmatrix}) = [\![\mathtt{x}]\!] \cdot (1 + |\alpha - \beta|^2).$$

- expectation q satisfies the above inequality and we obtain

$$\mathtt{qect}\Big[CT(\mathtt{q})\Big]\Big\{\underline{0}\Big\} \leqslant \mathtt{qect}\Big[\mathtt{x}^{\mathcal{B}} = \mathtt{true}\Big]\Big\{g\Big\}$$
$$= g[\mathtt{x} := 1] = \lambda(s, \begin{pmatrix} \alpha \\ \beta \end{pmatrix}).1 + |\alpha - \beta|^2$$

QPL: Classic Part



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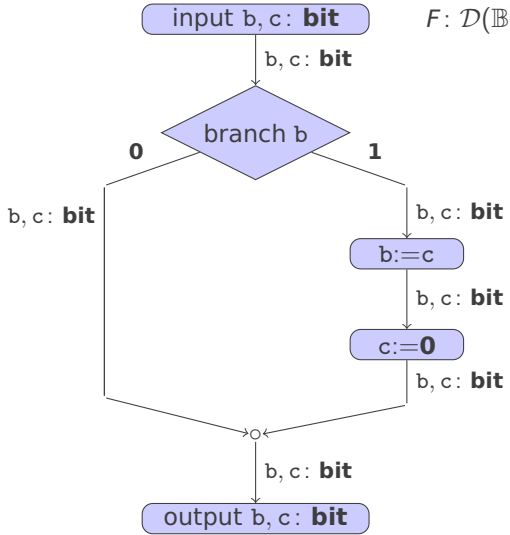
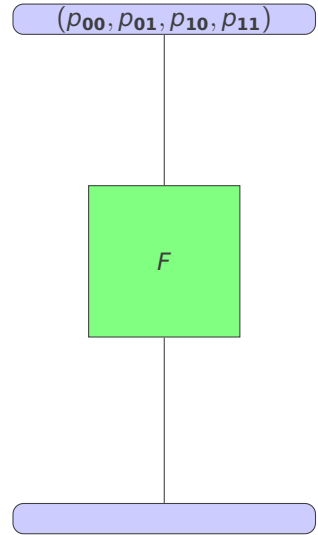
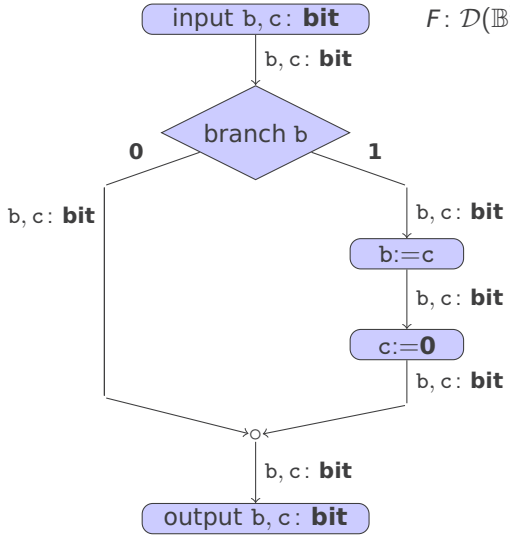


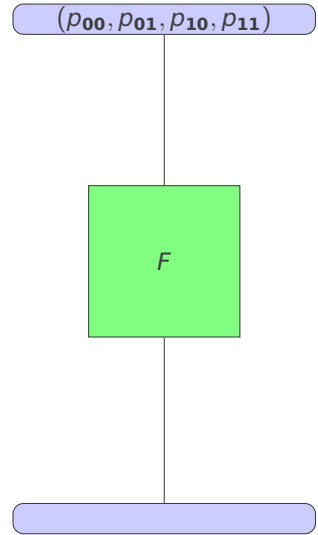
$F\colon \mathcal{D}(\mathbb{B}^2) \to \mathcal{D}(\mathbb{B}^2)$



QPL: Classic Part



$F\colon \mathcal{D}(\mathbb{B}^2) \to \mathcal{D}(\mathbb{B}^2)$



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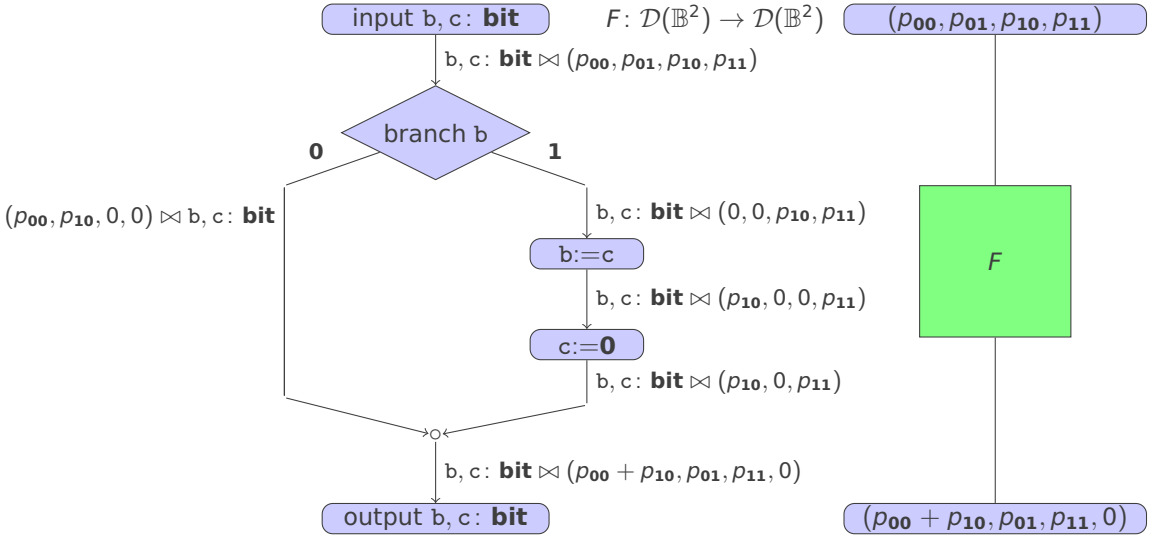
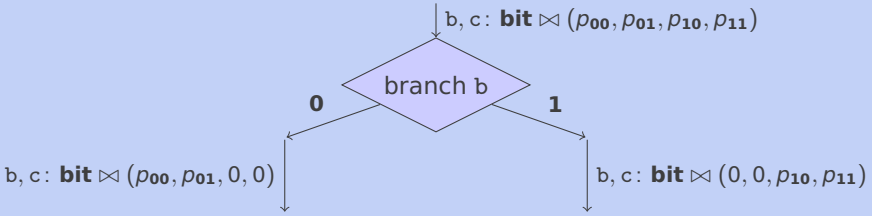


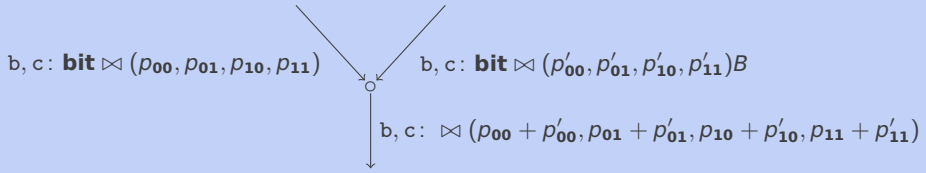
Classical Flow Charts

Branching



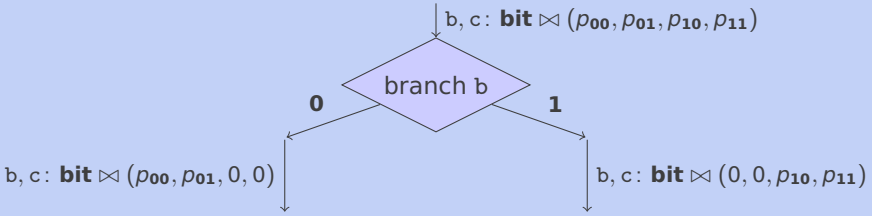
Classical Flow Charts

Merge



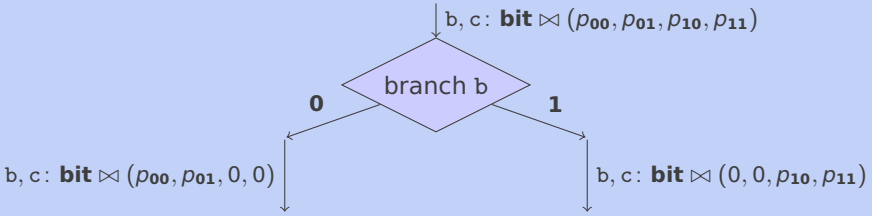
Classical Flow Charts

Branching



Classical Flow Charts

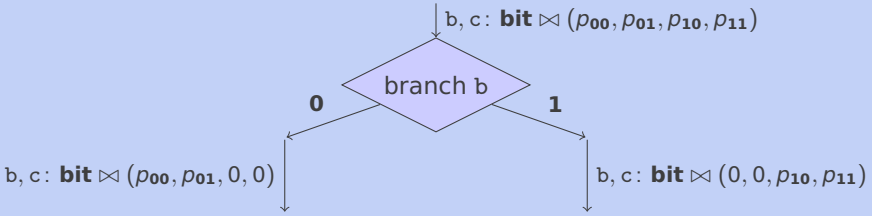
Branching



- a state of a program is a pair (e, σ)
  - e is an edge (conceivable as program location)
  - $\sigma : \mathcal{V} \to \mathbb{B}$ is a store

Classical Flow Charts

Branching



- a state of a program is a pair (e, σ)
  - e is an edge (conceivable as program location)
  - $\sigma : \mathcal{V} \to \mathbb{B}$ is a store
- observe that program locations and stores are interchangable:
  - program locations (aka program counters) are often just variables
  - different stores are representable by different control paths

Density Matrices & Löwner partial order

Definition

a density matrix is a positive Hermitian matrix A s.t. $tr(A) = 1$; a subdensity matrix is a positive Hermitian matrix A s.t. $tr(A) \leqslant 1$

Example

consider quantum state $|\varphi\rangle = \frac{1}{\sqrt{2}}|\mathbf{0}\rangle - \frac{1}{\sqrt{2}}|\mathbf{1}\rangle$, which is representable by the density matrix $|\varphi\rangle\langle\varphi|$:

$$|\varphi\rangle\langle\varphi| = \begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix}$$

let D_n denote the set of subdensity matrices of dimension n

Definition

for matrices $A, B \in D_n$, define $A \sqsubset B$, if $B - A$ is positive

Proposition

the partial order set $(D_n, \sqsupseteq)$ is a CPO, that is, every increasing sequence admits least upper bounds