



Séminaire Gallium
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Toward certified quantum programming

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Take away

- Quantum computers (are going to / will . . .) arrive
→ How to write correct programs?
- Need specification and verification mechanisms
 - scale invariant
 - close to quantum algorithm descriptions
 - well distinguished from code itself
 - largely automated
- We are developing *Qbricks* as a first step towards this goal
 - core building circuit language
 - dual semantics
 - high level specification framework
- Certified implementation of the phase estimation algorithm (quantum part of Shor)

Outline

Context

The case for verification of quantum algorithms

Qbricks

- Circuit language

- Dual semantics

- Derive proof obligations

- Toward further automation

Case study: phase estimation algorithm

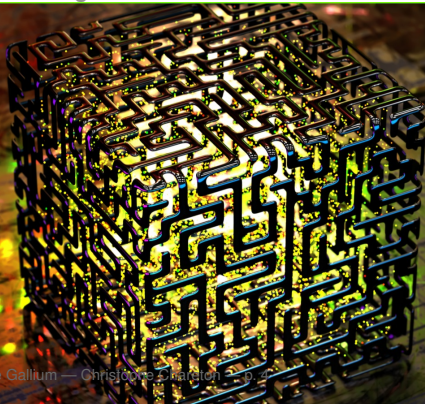
Conclusion

Dreams of quantum computing

MACHINES

How long until quantum computing is for everyone?

1 HOUR AGO 38 VIEWS



Applications:

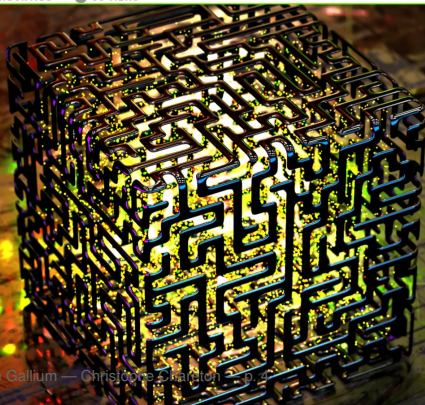
- Machine learning
- Chemistry
- Optimisation
- Cryptography
- Scheduling
- etc

Dreams of quantum computing

MACHINES

How long until quantum computing is for everyone?

1 HOUR AGO 38 VIEWS



If quantum mechanics hasn't profoundly shocked you, you haven't understood it yet.

(Niels Bohr)

izquotes.com



If you think you understand quantum mechanics, you don't understand quantum mechanics.

— Richard P. Feynman —

They are coming

IBM will soon launch a 53-qubit quantum computer

Frederic Lardinois @fredericl / 12:00 pm +00 • September 18, 2019



Google claims to have reached quantum supremacy

Researchers say their quantum computer has calculated an impossible problem for ordinary machines

They are coming

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Noisy Intermediate Scale Quantum (NISQ - J. Preskill 2018)

- Algorithm have to deal with noise
- Limited ressources :
 - 50 - 1000 qubits
 - limited circuit depth

Google claims to have reached quantum supremacy

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They are coming

IBM will soon launch a 53-qubit quantum

com Theoretical results:

- Computing gains Vs best-known classical algorithms:
 - Quantum walks: from linear to logarithmic
 - Grover-based searches: from e^n to $e^{\frac{n}{2}}$
 - Shor-like algorithms: from exponential to linear
 - Quantum simulation: from exponential to linear
- "Absolute" theoretical quantum supremacy?

$$\text{BQP} \stackrel{?}{\subseteq} \text{NP}$$

$$\text{BPP} \subseteq \text{BQP}$$

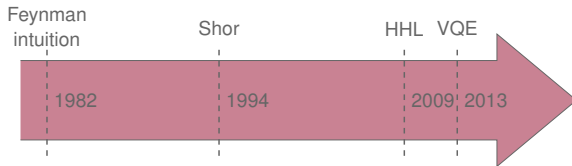
$$\text{BQP} \stackrel{?}{\supseteq} \text{NP}$$

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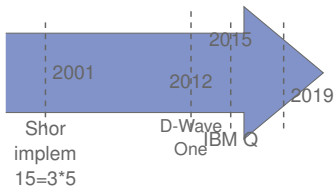
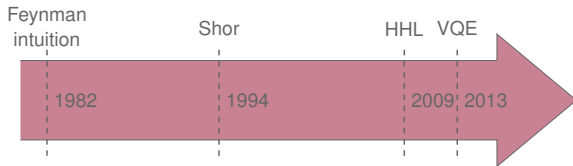
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Go
sup

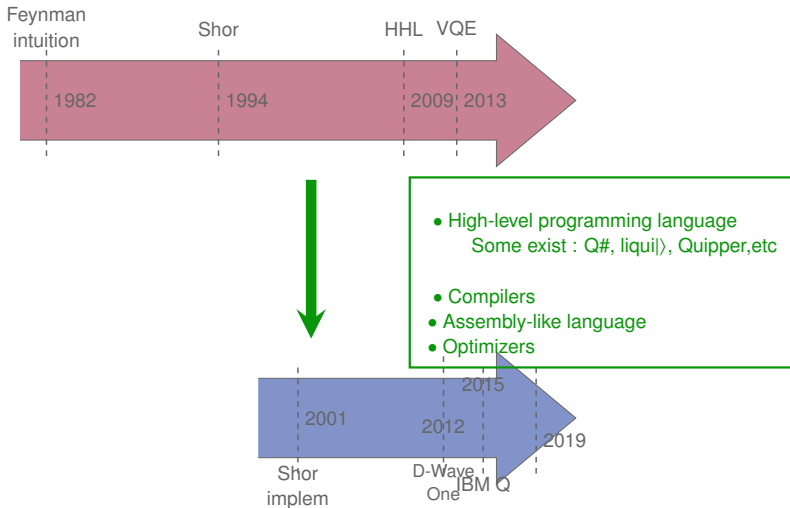
Quantum computing milestone history



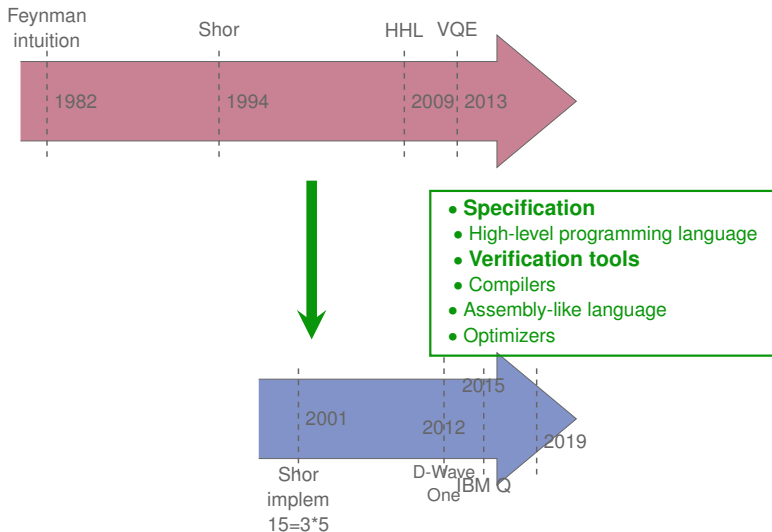
Quantum computing milestone history



Quantum computing milestone history



Quantum computing milestone history



Quantum information

- Classical world:



XOR



- Quantum world¹

 \oplus 

with $\alpha_0, \alpha_1 \in \mathbb{C}, |\alpha_0|^2 + |\alpha_1|^2 = 1$

¹In a 2^n dimension vector space, $|k\rangle_n$ designates the k^{th} canonical basis vector

Quantum information

■ Classical world:



One sequence in $\{\text{cat}, \text{X}\}^n$ (over 2^n possible)

■ Quantum world¹

$$|\alpha\rangle_n = \bigoplus_{k=0}^{2^n-1} \alpha_k |k\rangle_n = \bigoplus_{k=0}^{2^n-1} \alpha_k |k\rangle_n = \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \dots \\ \alpha_{2^n-1} \end{pmatrix}$$

¹In a 2^n dimension vector space, $|k\rangle_n$ designates the k^{th} canonical basis vector

Quantum information

■ Classical world:

₀
₁
₂
₃
 ...
 _{n-1}

One sequence in $\{\text{cat face}, \text{cat face with red X}\}^n$ (over 2^n possible)

■ Quantum world¹

$$|\alpha\rangle_n = \bigoplus \begin{array}{l} \alpha_0 \quad \text{cat face}_0 \text{ cat face}_1 \text{ cat face}_2 \text{ cat face}_3 \dots \text{cat face}_{n-1} \\ \alpha_1 \quad \text{cat face}_0 \text{ cat face}_1 \text{ cat face}_2 \text{ cat face}_3 \dots \text{cat face with red X}_{n-1} \\ \dots \\ \alpha_{2^n-1} \quad \text{cat face with red X}_0 \text{ cat face with red X}_1 \text{ cat face with red X}_2 \text{ cat face with red X}_3 \dots \text{cat face with red X}_{n-1} \end{array}$$

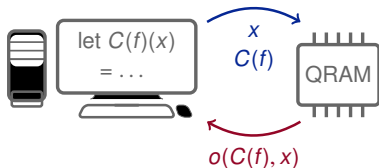
+ Some strange rules:

- no cloning
- destructive measure
- operations restricted to unitary

¹In a 2^n dimension vector space, $|k\rangle_n$ designates the k^{th} canonical basis vector

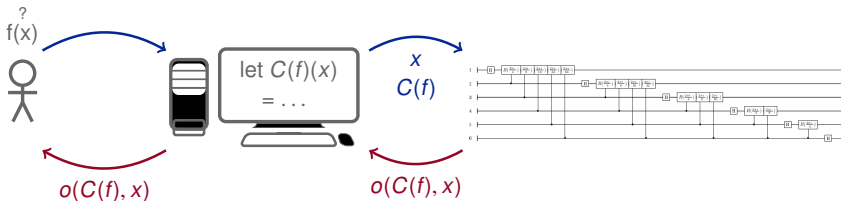
The QRAM model

- A quantum co-processor (QRAM), controlled by a classical computer
 - Classical control flow
 - Quantum computing request, sent to the QRAM
- → Structured sequences of instructions: quantum circuits



The QRAM model

- A quantum co-processor (QRAM), controlled by a classical computer
 - Classical control flow
 - Quantum computing request, sent to the QRAM
- → Structured sequences of instructions: quantum circuits



Does the circuit fit the computation need?

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Toward further automation

Case study: phase estimation algorithm

Conclusion

How do we check them?

implements

$|0\rangle|u\rangle$
 $\rightarrow \frac{1}{\sqrt{2^j}} \sum_{j=0}^{2^j-1} |j\rangle|u\rangle$
 $\rightarrow \frac{1}{\sqrt{2^j}} \sum_{j=0}^{2^j-1} |j\rangle U^j |u\rangle$
 $= \frac{1}{\sqrt{2^j}} \sum_{j=0}^{2^j-1} e^{2\pi i j \varphi_n} |j\rangle|u\rangle$
 $\rightarrow |\tilde{\varphi}_n\rangle|u\rangle$
 $\rightarrow \tilde{\varphi}_n$

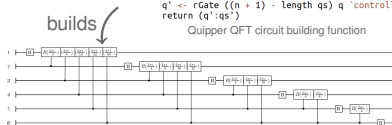
Quantum phase estimation (from Nielsen & Chuang)

initial state
 create superposition
 apply black box
 result of black box
 apply inverse Fourier transform
 measure first register

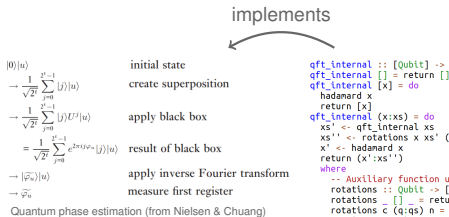
```

qft_internal :: [Qubit] -> Circ [Qubit]
qft_internal [] = return []
qft_internal [x] = do
  hadamard x
  return [x]
qft_internal (x:xs) = do
  xs' <- qft_internal xs
  xs'' <- rotations x xs' (length xs')
  x' <- hadamard x
  return (x':xs'')
where
  -- Auxiliary function used by 'qft'.
  rotations :: Qubit -> [Qubit] -> Int -> Circ [Qubit]
  rotations _ [] _ = return []
  rotations c (q:qs) n = do
    qs' <- rotations c qs n
    q' <- rGate ((n + 1) - length qs) q 'controlled' c
    return (q':qs')
        
```

Quipper QFT circuit building function



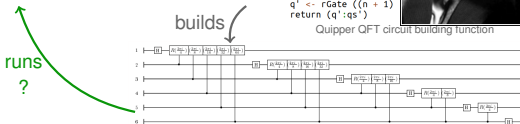
How do we check them?



If you think you understand quantum mechanics, you don't understand quantum mechanics.

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AZ QUOTES



- Quantum programming is tricky and non-intuitive
- No means to control an execution
- Tests are expensive and often statistical

How do we check them?

implements

$|0\rangle|u\rangle$ initial state

$-\frac{1}{\sqrt{2^n}} \sum_{j=0}^{2^n-1} |j\rangle|u\rangle$ create superposition

$-\frac{1}{\sqrt{2^n}} \sum_{j=0}^{2^n-1} |j\rangle U^j|u\rangle$ apply black box

$= \frac{1}{\sqrt{2^n}} \sum_{j=0}^{2^n-1} e^{2\pi i j \varphi_n} |j\rangle|u\rangle$ result of black box

$-\frac{1}{\sqrt{2^n}} |\varphi_n\rangle|u\rangle$ apply inverse Fourier transform

$-\frac{1}{\sqrt{2^n}} \varphi_n$ measure first register

Quantum phase estimation (from Nielsen & Chuang)

```

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    return (q':qs')
    
```

Quipper QFT circuit building function

builds

runs ?

- Testing is difficult ...
- What about full verification? allows to handle
 - Infinite state space
 - absolute guarantee

[A parte] Annotated code and deductive verification



- Provides absolute guarantee
- Automates proofs
- Industrial successes
- Verify wide-spread languages (C, Java, caml . . .)



Three main ingredients:

- operational semantics
- specification language
- proof engine



State of affairs in quantum computing

Three main ingredients:

- operational semantics: matrices \rightarrow matrix product, from Heisenberg (1925), Dirac (1939) path-sums (2018)
- specification language: ???
- proof engine: ???

Our strategy

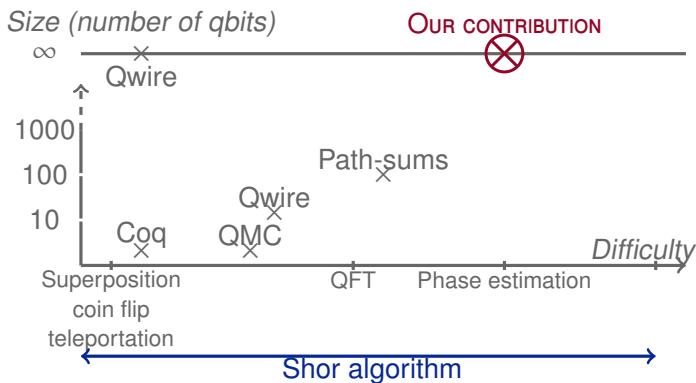
- Build on best practice of formal verification for the classical case
 - separation of concerns
 - scale invariant verification
 - proof automation
 - domain-based specialization
 - flexible specification language
- Tailor them to the quantum case
 - dual semantics (truth reference + specifications)
 - specific reasoning rules
 - dedicated lemmas (1000+) libraries

State of the art

	QMC	Coq	Qwire (Coq)	Path-sums	Qbricks
• Separate specification from code	✓	✗	✓	✗	✓
• Scale invariance	✗	✓	✓	✗	✓
• Specifications fitting algorithm	✗	✗	✗	✓	✓
• Automate proofs	✓	✗	✗	✓	➔

Table: Formal verification of quantum circuits

State of the art, achievements in quantum formal verification



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The quantum case : Back to basics

1. $|0\rangle|u\rangle$ initial state
2. $\rightarrow \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} |j\rangle|u\rangle$ create superposition
3. $\rightarrow \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} |j\rangle U^j |u\rangle$ apply black box
 $= \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} e^{2\pi i j \varphi_u} |j\rangle|u\rangle$ result of black box
4. $\rightarrow |\widetilde{\varphi}_u\rangle|u\rangle$ apply inverse Fourier transform
5. $\rightarrow \widetilde{\varphi}_u$ measure first register

Algorithm for the quantum phase estimation

The quantum case : Back to basics

1. $|0\rangle|u\rangle$
2. $\rightarrow \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} |j\rangle|u\rangle$
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4. $\rightarrow |\widetilde{\varphi}_u\rangle |u\rangle$
5. $\rightarrow \widetilde{\varphi}_u$

initial state
create superposition

apply black box

result of black box

apply inverse Fourier transform
measure first register

- A sequence of operations
- Intermediate assertions, describing the state of the system at each step

Algorithm for the quantum phase estimation

The quantum case : Back to basics

1.	$ 0\rangle u\rangle$
2.	$\rightarrow \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} j\rangle u\rangle$
3.	$\rightarrow \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} j\rangle U^j u\rangle$ $= \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} e^{2\pi i j \varphi_u} j\rangle u\rangle$
4.	$\rightarrow \widetilde{\varphi}_u\rangle u\rangle$
5.	$\rightarrow \widetilde{\varphi}_u$

initial state

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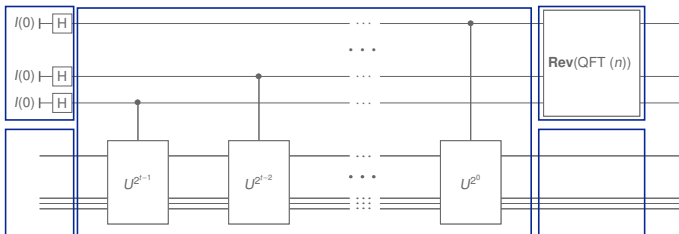
Algorithm for the quantum phase estimation

Derive function specifications, eg :

let `create_superposition (state)`*pre: |u> is a ket vector**pre: state = |0>|u>**post: state = $\frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} |j\rangle|u\rangle$* *= (* The program *)*

- Deductive verification (of annotated programs)
- → a domain specific language, embedded in the Why3 environment
 - *build on best practice for the classical case (automation, separation of concerns, ...)*
 - + interface with SMT-solvers

Circuit building functions



```
type quantum_circuit_pre =  
  Phase real | Rx real | Ry real | Rz_real | Cnot  
  | Sequence quantum_circuit_pre quantum_circuit_pre  
  | Parallel quantum_circuit_pre quantum_circuit_pre
```

Specification and verification

- Decorate *Qbricks* code with specifications
- Interprete circuit as functions transforming quantum states

x : quantum_state semantics
 C : quantum_circuit \longrightarrow $\llbracket C, x \rrbracket$: quantum_state

- Path-sum semantics, general form

$$C, |k\rangle_n \xrightarrow{\text{path_sum_sem}} \frac{1}{\sqrt{2^r}} \sum_{j=0}^{2^r-1} \text{ph}(k, j) |\text{ket}(i, j)\rangle_n$$

- Three separated parameters, with recursive definitions:
 - r : int
 - $\text{ph} : \text{int} \rightarrow \text{int} \rightarrow \text{complex}$
 - $\text{ket} : \text{int} \rightarrow \text{int} \rightarrow \text{int}$

Specified circuit building

- Three separated parameters:
 - r : int
 - ph : int \rightarrow int \rightarrow complex
 - ket : int \rightarrow int \rightarrow int
- functions r (sum_range), ph ($phase_part$) and ket (ket_part) are defined by recursion for circuits,

```

let rec function ket_part (c:quantum_circuit) (bv_x bvy: int -> int) (i: int)
= match to_pre c with
  | Phase_ _ -> bv_x i
  | Rx_ _ -> bvy i
  | Ry_ _ -> bvy i
  | Rz_ _ -> bv_x i
  | Cnot -> if i = 1 then mod (bv_x 0 + bv_x 1) 2 else bv_x i
  | Sequence_ d e ->
    ket_part (to_qc e) (ket_part (to_qc d) bv_x bvy) (shift bvy (sum_range (to_qc d))) i
  | Parallel_ d e -> (concat_fun (ket_part (to_qc d) bv_x bvy)
    (ket_part (to_qc e) (shift bv_x (depth (to_qc d)))
    (shift bvy (sum_range (to_qc d)))) (depth (to_qc d))) i

let rec function phase_part (c:quantum_circuit) (bv_x bvy: int -> int) ...
let rec function sum_range (c:quantum_circuit) (bv_x bvy: int -> int) ...
let function path_sum_sem (c:quantum_circuit) (x: matrix t)
= ...
(pow_inv_sqrt_2 (sum_range c)) *.. mat_sum (n_bvs (sum_range c)
(fun bvy -> phase_part (ket_to_bv x) bvy)*.. (bv_to_ket ket_part (ket_to_bv x) bvy)))

```

Specified circuit building

- Three separated parameters:

- r : int
- ph : $\text{int} \rightarrow \text{int} \rightarrow \text{complex}$
- ket : $\text{int} \rightarrow \text{int} \rightarrow \text{int}$

- functions r (sum_range), ph (phase_part) and ket (ket_part) are defined by recursion for circuits,

- they specify circuit *lifted constructors*

```

let function sequence (d e: quantum_circuit): quantum_circuit
  requires {size d = size e}
  ensures {sum_range result = sum_range d + sum_range e}
  ensures {size result = size d}
  ensures {forall bvx bvy: int->int. forall i :int.
    ket_part result bvx bvy i = if 0<= i < size result then
      ket_part e (ket_part d bvx bvy) (shift bvy (sum_range d)) i else 0}
  ensures {forall bvx bvy: int->int. phase_part result bvx bvy =
    (phase_part d bvx bvy) *.
    (phase_part e (ket_part d bvx bvy) (shift bvy (sum_range d))) }
  = {to_pre = Sequence (to_pre d) (to_pre e)}

```

Specified circuit building

- Three separated parameters:
 - r : int
 - ph : int \rightarrow int \rightarrow complex
 - ket : int \rightarrow int \rightarrow int
- functions r (`sum_range`), ph (`phase_part`) and ket (`ket_part`) are defined by recursion for circuits,
- they specify circuit *lifted constructors*
- and the circuit building functions

```
let function hadamard(): quantum_circuit
  ensures {size result = 1}
  ensures {sum_range result = 1}
  ensures {forall bvx bvy: int-> int, forall i :int.
    0 <= i < size result -> ket_part result bvx bvy i = bvy i}
  ensures {forall bvx bvy: int-> int, binary bvx -> binary bvy ->
    phase_part result bvx bvy = value (dyadic (bvx 0 * bvy 0) 1) }
  =
  sequence (rzp 1) (ry (dyadic 1 3))
```

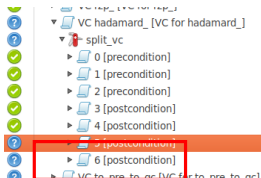
Generating proof obligations (why3)

■ Compilation generates proof obligations

```

let function hadamard(): quantum_circuit
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  ensures{forall bvx bvy: int-> int. binary bvx -> binary bvy ->
    phase_part result bvx bvy = value (dyadic (bvx 0 * bvy 0) 1)}
sequence (rzp 1) (ry (dyadic 1 3))

```



```

474
475 constant bvy : int -> int
476
477 constant i : int
478
479 axiom H1 : 0 <= i
480
481 axiom H : i < depth_result
482
483 ----- goal
484
485 goal VC hadamard_ : ket_part_result bvx bvy i = (bvy @ i)
486
487

```

Generating proof obligations (why3)

- Compilation generates proof obligations
- Calling a function provides its postconditions as axioms

```

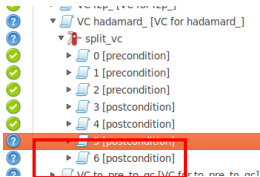
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  ensures{forall bvx bvy: int-> int. forall
    0<= i < size result -> ket_part result
    ensures{forall bvx bvy: int-> int. binary
      phase_part result bvx bvy = value
        =
        sequence (rzp 1) (ry (dyadic 1 3))
  }

```

```

493 axiom H7 :
494   forall bvx1:int -> int, bvy1:int -> int.
495   forall i1:int.
496     ket_part_result bvx1 bvy1 i1
497     = (if 0 <= i1 /\ i1 < depth_result
498       then ket_part_ry (dyadic 1 3))
499       (((fun (y0:quantum_circuit) (y1:int -> int) (y2:int -> int) (y3:
500         int) -> ket_part_y0 y1 y2 y3)
501         @ rzp_1)
502         @ bvx1)
503         @ bvy1)
504         (((fun (y0:int -> int) (y1:int) (y2:int) -> shift y0 y1 y2)
505           @ bvy1)
506           @ sum_range_(rzp_1))
507         i1
508       else 0)

```



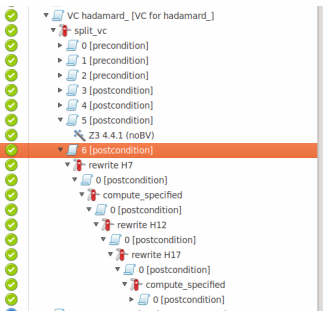
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Supporting proof obligations

- Proof obligations may be sent to SMT-solvers,
- and they can be eased, if needed, by to interactive transformations



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Path-sum semantics nice properties

- Path-sum semantics satisfies nice properties

Lemma (Properties of function \mathbf{Ps})

- **Linear decomposition.** Let c be a quantum circuit, then for any ket $|u\rangle$ of length s_c ,

$$\mathbf{Ps}(c, |u\rangle) = \sum_{k=0}^{2^{s_c}-1} (u(k)) \mathbf{Ps}(c, |k\rangle_{s_c})$$

- **Compositions.** Let c and c' be quantum circuits, let $|u\rangle$ and $|u'\rangle$ be ket of respective lengths s_c and $s_{c'}$. Then,
 - $\mathbf{Ps}(\text{parallel}(c, c'), |u\rangle \otimes |u'\rangle) = (\mathbf{Ps}(c, |u\rangle) \otimes (\mathbf{Ps}(c', |u'\rangle))$
 - if c and c' have the same size then $\mathbf{Ps}(\text{sequence}(c, c'), |u\rangle) = \mathbf{Ps}(c', \mathbf{Ps}(c, |u\rangle))$

- They enable local reasoning without reference to r , ph and ket

Abstract specification: the *eigen* example

Definition (Eigen predicate)

Let c be a quantum circuit, then for any ket $|u\rangle$ of length \mathbf{s}_c and for any complex number v , we say that $|u\rangle$ is an *eigenvector* for c with associated eigenvalue v , and we write $\text{eigen}(c, |u\rangle, v)$, iff

$$\mathbf{Ps}(c, |u\rangle) = v|u\rangle$$

Lemma (Eigen sequence composition)

Let c and c' be quantum circuits such that $\mathbf{s}_c = \mathbf{s}_{c'}$, let $|u\rangle$ be a ket of length \mathbf{s}_c . Then for any complex values v, v' such that

- $\text{eigen}(c, |u\rangle, v)$
- $\text{eigen}(c', |u\rangle, v')$

then

$$\text{eigen}(\text{sequence}(c, c'), |u\rangle, vv')$$

Abstract specification and quantum algorithms

- Quantum algorithms (phase estimation, Grover, quantum simulation, etc.) are often parametrized by an *oracle* quantum circuit, respecting a given property
- This specification may not (nicely) translate in terms of r , ph and ket
- → abstract specifications
- Example, the phase estimation algorithm:
 - Input:** an unitary operator U and an eigenstate $|v\rangle$ of U
 - Output:** the eigenvalue associated to $|v\rangle$
- Also: reversed circuit specification, controlled operations specifications, bit permutation specifications, etc.

Specific language fragments and simplified path-semantics

- Predicates may characterize *Qbricks* fragments with simplified path-sum semantics:

Spec.	generating syntax	Semantics	Design input
\top	{Rx, Ry, Rz, Ph, Cnot}	$r: \text{int}$ $ph: \text{int} \rightarrow \text{int} \rightarrow \text{complex}$ $ket: \text{int} \rightarrow \text{int} \rightarrow \text{int}$	
flat	{Rz, Ph, Cnot}	$ph: \text{int} \rightarrow \text{complex}$ $ket: \text{int} \rightarrow \text{int}$	easy specification
diag	{Rz, Ph}	$ph: \text{int} \rightarrow \text{complex}$	easier specification iterators

Outline

Context

The case for verification of quantum algorithms

Qbricks

Circuit language

Dual semantics

Derive proof obligations

Toward further automation

Case study: phase estimation algorithm

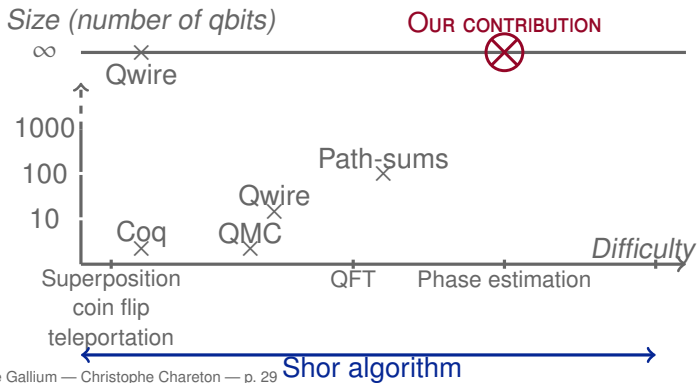
Conclusion

Phase estimation

Input: an unitary operator U and an eigenstate $|v\rangle$ of U

Output: the eigenvalue associated to $|v\rangle$

- Eigen decomposition
- Solving linear systems
- Shor (with arithmetic assumption and probability)



Implementation data

	#Lines	#Def.	#Lem	#POs	#Aut.	#Cmd
<i>create_superposition</i>	42	2	1	11	6	36
<i>apply_black_box</i>	57	3	1	50	44	46
QFT	75	3	0	57	51	30
<i>phase estimation</i>	63	4	0	72	65	51
Total	237	12	2	190	166	163

#Aut.: automatically proven POs — #Cmd: interactive commands

Table: Implementation & verification of phase estimation

- The objective is reached: prove by fact that parametrized formal verification for quantum programs is possible
- Future works : further automate proof fulfillment

Comparison of several approaches, QFT algorithm


	QMC	Coq	Qwire (Coq)	Path-sums	Qbricks
• Separate specification from code	✓	✗	✓	✗	✓
• Scale invariance	✗	✓	✓	✗	✓
• Specifications fitting algorithm	✗	✗	✗	✓	✓
• Automate proofs	✓	✗	✗	✓	✓ 

Table: Formal verification of quantum circuits

	#Lines	#Def.	#Lem	#POs	#Aut.	#Cmd
QFT (full <i>Qbricks</i>)	75	3	0	57	51	30
QFT (Path-sum only)	87	3	0	73	64	49
QFT (Matrix only, cf QMC, Coq solutions)	200	8	15	306	285	106

Table: Comparison of several approaches, QFT algorithm

Conclusion

- *Qbricks*: a core development framework for certified quantum programming
 - scale invariant
 - close to quantum algorithm descriptions
 - well distinguished from code itself
 - largely automated
- Implementation
 - Circuit building language
 - Dual semantics + equivalence proof
 - Shortcuts for further automation
 - Certified implementation of the phase estimation algorithm
- Future works:
 - Further automate proof framework
 - Extend *Qbricks* to measure → Shor

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