

Generating Formally Verified Quantum Fourier Transform Algorithms

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- Formally verified mapping from matrix specifications to quantum circuits
- Alternative circuits generated using verified rewrite rules corresponding to matrix factorizations
 - Matrix factorizations encoded and derived using SPIRAL methodology.
- Verification using the Coq Proof Assistant
 - Quantum circuits defined by SQIR programs
 - Matrix semantics supported by QuantumLib with extensions

- ① Quantum Computing
- ② The Discrete Fourier Transform and Quantum Fourier Transform
- ③ Generating Quantum Algorithms
- ④ Formal Verification
- ⑤ Future Work

Qubit

- Quantum State
 - 2-dimensional Complex Hilbert Space
 - $|0\rangle = e_0^2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|1\rangle = e_1^2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$
- Superposition
 - $\alpha |0\rangle + \beta |1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ with $|\alpha|^2 + |\beta|^2 = 1$
- Measurement
 - States $|0\rangle$ and $|1\rangle$ with probability $|\alpha|^2$ and $|\beta|^2$

Multi-Qubit System

- Tensor Product

- $e_i^m \otimes e_j^n = e_{in+j}^{mn}$

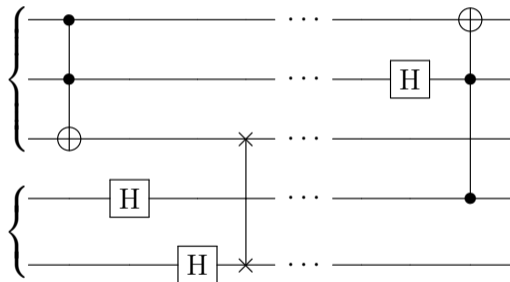
- $|00\rangle = |0\rangle \otimes |0\rangle = e_0^4 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \dots, |11\rangle = |1\rangle \otimes |1\rangle = e_3^4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$

- Preserves norm condition
- Pure versus entangled

Quantum Circuits (without measurement)

- Unitary Operators
 - Must preserve norm
 - $UU^\dagger = I_n$
- Implemented with quantum gates
- Not all Unitary operations have the same costs

Quantum Circuit



Quantum Gates


- Hadamard Gate — \boxed{H} —

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

- Phase Shift Gate — $\boxed{P_{\exp(i\phi)}}$ —

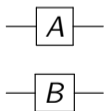
- $\begin{bmatrix} 1 & \\ & \exp(i\phi) \end{bmatrix}$

Quantum Gates

- SWAP gate 
 - $|q_0 q_1\rangle \mapsto |q_1 q_0\rangle$
 - $$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$
- General SWAP_{m,n}
 - $|q_0 \dots q_m \dots q_n \dots\rangle \mapsto |q_0 \dots q_n \dots q_m \dots\rangle$
 - Can be decomposed into multiple simple SWAPs.

Tensor (Kronecker) Product

- $(A \otimes B)(x \otimes y) = Ax \otimes By$
 - Associative (Not Commutative)
 - $(A \otimes B)(C \otimes D) = AC \otimes BD$
 - $(A \otimes B) = (A \otimes I)(I \otimes B) = (I \otimes B)(A \otimes I)$
 - $I_m \otimes I_n = I_{mn}$
- Parallel Gate Application



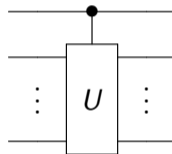
$$A^{2 \times 2} \otimes B^{2 \times 2} =$$

$$\begin{bmatrix} a_{00}b_{00} & a_{00}b_{01} & a_{01}b_{00} & a_{01}b_{01} \\ a_{00}b_{10} & a_{00}b_{11} & a_{01}b_{10} & a_{01}b_{11} \\ a_{10}b_{00} & a_{10}b_{01} & a_{11}b_{00} & a_{11}b_{01} \\ a_{10}b_{10} & a_{10}b_{11} & a_{11}b_{10} & a_{11}b_{11} \end{bmatrix}$$

Quantum Gates

- Controlled Gates

- Applies U to *target* qubits when *source* qubit is $|1\rangle$.
- Notation CU for gates controlled by the leading qubit
- $CU^{n \times n} = |0\rangle\langle 0| \otimes I_n + |1\rangle\langle 1| \otimes U = I_n \oplus U$
 - $\langle x| = |x\rangle^\dagger$



Quantum Fourier Transform

Discrete Fourier Transform

Let $\omega = \exp(\frac{2\pi i}{n})$ be a primitive n^{th} root of unity. The n -point Discrete Fourier Transform is the matrix vector product $y = \text{DFT}_n x$ where

$$\text{DFT}_n e_j^n = \sum_{j=0}^{n-1} \omega^{ij} e_j^n.$$

- $\text{DFT}_n = \begin{bmatrix} 1 & 1 & \dots & 1 \\ 1 & \omega & \dots & \omega^{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{n-1} & \dots & \omega^{(n-1)(n-1)} \end{bmatrix}$
- $\text{DFT}_n^{-1} = \frac{1}{n} \text{DFT}_n(\bar{\omega})$

Quantum Fourier Transform

- Normalized Discrete Fourier Transform
- QFT on n qubits is $\frac{1}{\sqrt{2^n}} \text{DFT}_{2^n}$
- $\text{QFT}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \text{H}$

Recursive Cooley-Tukey Factorization

$$\text{DFT}_{rs} = (\text{DFT}_r \otimes \text{I}_s) \text{T}_s^{rs} (\text{I}_r \otimes \text{DFT}_s) \text{L}_r^{rs}$$

$$\text{DFT}_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & i & 1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & 1 & i \end{bmatrix} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & i \end{bmatrix} \begin{bmatrix} 1 & 1 & & \\ 1 & -1 & & \\ & & 1 & 1 \\ & & 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$

$$\text{DFT}_4 = (\text{DFT}_2 \otimes \text{I}_2) \text{T}_2^4 (\text{I}_2 \otimes \text{DFT}_2) \text{L}_2^4$$

Stride Permutations

- $L_n^{mn}(e_i^m \otimes e_j^n) = e_j^n \otimes e_i^m$
- Circular shift of qubits
- $L_2^4 = \text{SWAP}$

Generating Quantum Algorithms

DFT_{16}

$$= (\text{DFT}_2 \otimes \text{I}_8) \text{T}_8^{16} (\text{I}_2 \otimes \text{DFT}_8) \text{L}_2^{16}$$

$$= (\text{DFT}_2 \otimes \text{I}_8) \text{T}_8^{16} (\text{I}_2 \otimes (\text{DFT}_2 \otimes \text{I}_4) \text{T}_4^8 (\text{I}_2 \otimes \text{DFT}_4) \text{L}_2^8) \text{L}_2^{16}$$

$$= (\text{DFT}_2 \otimes \text{I}_8) \text{T}_8^{16} (\text{I}_2 \otimes (\text{DFT}_2 \otimes \text{I}_4) \text{T}_4^8 (\text{I}_2 \otimes ((\text{DFT}_2 \otimes \text{I}_2) \text{T}_2^4 (\text{I}_2 \otimes \text{DFT}_2) \text{L}_2^4)) \text{L}_2^8) \text{L}_2^{16}$$

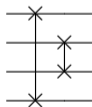
$$= (\text{DFT}_2 \otimes \text{I}_8) \text{T}_8^{16} (\text{I}_2 \otimes \text{DFT}_2 \otimes \text{I}_4) (\text{I}_2 \otimes \text{T}_4^8) (\text{I}_4 \otimes \text{DFT}_2 \otimes \text{I}_2) (\text{I}_4 \otimes \text{T}_2^4) (\text{I}_8 \otimes \text{DFT}_2) \\ \times (\text{I}_4 \otimes \text{L}_2^4) (\text{I}_2 \otimes \text{L}_2^8) \text{L}_2^{16}$$

$$= (\text{DFT}_2 \otimes \text{I}_8) \text{T}_8^{16} (\text{I}_2 \otimes \text{DFT}_2 \otimes \text{I}_4) (\text{I}_2 \otimes \text{T}_4^8) (\text{I}_4 \otimes \text{DFT}_2 \otimes \text{I}_2) (\text{I}_4 \otimes \text{T}_2^4) (\text{I}_8 \otimes \text{DFT}_2) \text{R}_{24}$$

Generating Quantum Algorithms

Bit Reversal

- $R_{2^n}(e_{i_0}^2 \otimes e_{i_1}^2 \otimes \cdots \otimes e_{i_{n-1}}^2) = (e_{i_{n-1}}^2 \otimes e_{i_{n-2}}^2 \otimes \cdots \otimes e_{i_0}^2)$
- $R_{2^n} = (I_2 \otimes R_{2^{n-1}})L_2^{2^n}$
- Flips the order of qubits
- Can be implemented using telescoping SWAPs



Generating Quantum Algorithms

DFT_{16}

$$\begin{aligned} &= (\text{DFT}_2 \otimes \text{I}_8) \text{T}_8^{16} (\text{I}_2 \otimes \text{DFT}_2 \otimes \text{I}_4) (\text{I}_2 \otimes \text{T}_4^8) (\text{I}_4 \otimes \text{DFT}_2 \otimes \text{I}_2) (\text{I}_4 \otimes \text{T}_2^4) (\text{I}_8 \otimes \text{DFT}_2) \\ &\quad \times (\text{I}_4 \otimes \text{L}_2^4) (\text{I}_2 \otimes \text{L}_2^8) \text{L}_2^{16} \\ &= (\text{DFT}_2 \otimes \text{I}_8) \text{T}_8^{16} (\text{I}_2 \otimes \text{DFT}_2 \otimes \text{I}_4) (\text{I}_2 \otimes \text{T}_4^8) (\text{I}_4 \otimes \text{DFT}_2 \otimes \text{I}_2) (\text{I}_4 \otimes \text{T}_2^4) (\text{I}_8 \otimes \text{DFT}_2) \\ &\quad \times (\text{I}_2 \otimes (\text{I}_2 \otimes \text{L}_2^4) \text{L}_2^8) \text{L}_2^{16} \\ &= (\text{DFT}_2 \otimes \text{I}_8) \text{T}_8^{16} (\text{I}_2 \otimes \text{DFT}_2 \otimes \text{I}_4) (\text{I}_2 \otimes \text{T}_4^8) (\text{I}_4 \otimes \text{DFT}_2 \otimes \text{I}_2) (\text{I}_4 \otimes \text{T}_2^4) (\text{I}_8 \otimes \text{DFT}_2) \\ &\quad \times (\text{I}_2 \otimes \text{R}_{2^3}) \text{L}_2^{16} \\ &= (\text{DFT}_2 \otimes \text{I}_8) \text{T}_8^{16} (\text{I}_2 \otimes \text{DFT}_2 \otimes \text{I}_4) (\text{I}_2 \otimes \text{T}_4^8) (\text{I}_4 \otimes \text{DFT}_2 \otimes \text{I}_2) (\text{I}_4 \otimes \text{T}_2^4) (\text{I}_8 \otimes \text{DFT}_2) \text{R}_{2^4} \end{aligned}$$

Generating Quantum Algorithms

Twiddle Factors

- $T_n^{mn}(\omega) = \begin{bmatrix} I_n & & & \\ & \Omega_n(\omega) & & \\ & & \ddots & \\ & & & \Omega^{m-1}(\omega) \end{bmatrix}$

- $\Omega_n(\omega) = \text{diag}(1, \omega, \omega^2, \dots, \omega^{n-1})$

- Some properties

- $\Omega_2(\omega) = P_\omega$

- $C(U_1 U_2) = (C U_1)(C U_2)$

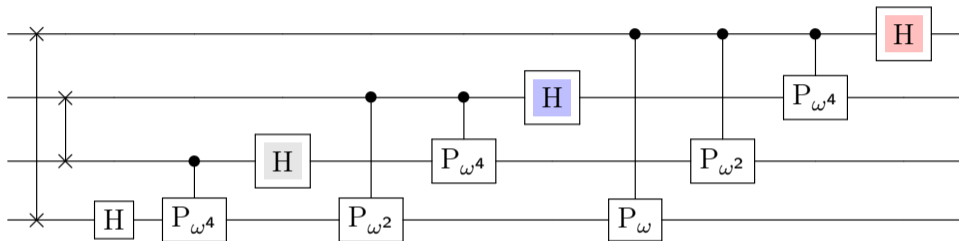
- $\Omega_n^k(\omega) = \Omega_n(\omega^k)$

- $\Omega_{2n}(\omega) = \Omega_2^n(\omega) \otimes \Omega_n(\omega)$

$$\begin{aligned}T_8^{16}(\omega) &= \begin{bmatrix} I_8 & \\ & \Omega_8(\omega) \end{bmatrix} \\ &= C\Omega_8(\omega) \\ &= C(\Omega_2^4(\omega) \otimes \Omega_4(\omega)) \\ &= C(\Omega_2^4(\omega) \otimes (\Omega_2^2(\omega) \otimes \Omega_2(\omega))) \\ &= C(\Omega_2(\omega^4) \otimes \Omega_2(\omega^2) \otimes \Omega_2(\omega)) \\ &= C(P_{\omega^4} \otimes P_{\omega^2} \otimes P_{\omega}) \\ &= C((P_{\omega^4} \otimes I_4)(I_2 \otimes P_{\omega^2} \otimes I_2)(I_4 \otimes P_{\omega})) \\ &= C(P_{\omega^4} \otimes I_4)C(I_2 \otimes P_{\omega^2} \otimes I_2)C(I_4 \otimes P_{\omega})\end{aligned}$$

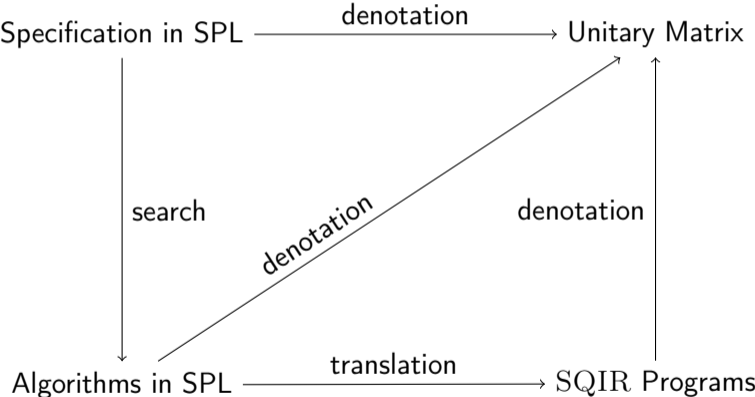
Generating Quantum Algorithms

Example breakdown: 4-qubit QFT



DFT_{16}

$$\begin{aligned}
 &= (\text{H} \otimes \text{I}_8)(\text{C}(\text{P}_{\omega^4} \otimes \text{I}_4))(\text{C}(\text{I}_2 \otimes \text{P}_{\omega^2} \otimes \text{I}_2))(\text{C}(\text{I}_4 \otimes \text{P}_{\omega})) \\
 &\times (\text{I}_2 \otimes \text{H} \otimes \text{I}_4)(\text{I}_2 \otimes \text{C}(\text{P}_{\omega^4} \otimes \text{I}_2))(\text{I}_2 \otimes \text{C}(\text{I}_2 \otimes \text{P}_{\omega^2})) \\
 &\times (\text{I}_4 \otimes \text{H} \otimes \text{I}_2)(\text{I}_4 \otimes \text{C}\text{P}_{\omega^4}) \\
 &\times (\text{I}_8 \otimes \text{H})(\text{I}_2 \otimes \text{SWAP} \otimes \text{I}_2)\text{SWAP}_{0,3}
 \end{aligned}$$



QFT₄

Unitary Matrix Specification

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

Matrix Factorization in SPL

$$(H \otimes I_2)CP_i(I_2 \otimes H)SWAP$$

Algorithm mapped to SQIR

```
SWAP 0 1;  
H 1;  
control 0 (Rz i 1);  
H 0
```

Formal Verification done in the Coq Proof Assistant

- Encoding the abstract syntax of the necessary SPL subset as inductive data type (deep embedding)
- Unitary Matrix Semantics for SPL subset
- Rewrite Rules with self-contained proofs of correctness
 - Recursive Cooley-Tukey
 - Iterative Cooley-Tukey
- Verified simple search process
- Verified SPL to SQIR translation

SPL Embedding

Inductive $spl : nat \rightarrow Set :=$

| $spl_I : \forall n, spl\ n$

(* Non-terminal *)

| $spl_F : \forall n, spl\ n$

| $spl_T : \forall r\ s, spl\ (r+s)$

| $spl_L : \forall r\ s, spl\ (r+s)$

| $spl_Rev : \forall n, spl\ n$

(* Intermediary *)

| $spl_T' : \forall r\ s\ (k : nat), spl\ (r+s)$

| $spl_Omega : \forall n\ (k : nat), spl\ n$

(* Gates *)

| $spl_H : spl\ 1$

| $spl_P : nat \rightarrow spl\ 1$

| $spl_SWAP : spl\ 2$

| $spl_GSWP : \forall (dim\ m\ n : nat), spl\ dim$

...

(* Controlled Unitary *)

| $spl_C : \forall \{n\}, spl\ n \rightarrow spl\ (1 + n)$

(* $s_1 \times s_2$ *)

| $spl_comp : \forall \{n\} (s1 : spl\ n) (s2 : spl\ n), spl\ n$

(* $s_1 \otimes s_2$ *)

| $spl_kron : \forall \{n1\ n2\} (s1 : spl\ n1) (s2 : spl\ n2),$
 $spl\ (n1+n2)$

(* Equal-size casts with proof *)

| $spl_cast : \forall \{n1\ n2\} (Heq : n1 = n2) (s : spl\ n1),$
 $spl\ n2.$

with notations (not shown)

Rewrite Rules

- Dependent Records
 - Takes a left-hand-side SPL term
 - A number of degrees of freedom with constraints
 - The right-hand-side term
 - Proof that both sides are equal under constraints
 - A way to generate all possible right-hand-sides
 - Proofs that this generation is sound and complete
- Everything you need to know about a rule is in one place!
- Correctness proof of search is mechanical

```
Record rule {n} (r_lhs : spl n) :=
  mkRule
    { r_dof : nat
    ; r_constraint : nary Prop r_dof (* r_dof-ary predicate *)
    ; r_rhs : rule_rhs n r_dof r_constraint
    ; r_gen : list (gen_pair r_dof) (* every possible combination of parameters *)
    ; r_correct : rule_correct _ r_constraint r_lhs r_rhs (* correct w.r.t constraint *)

  (* Generation produces every correct set of parameters *)
    ; r_gen_sound : Forall (constraint_holds r_constraint) (r_gen)
    ; r_gen_complete :  $\forall p$ , (constraint_holds r_constraint p)  $\rightarrow$  In p r_gen
    }.
```

Cooley-Tukey Rule

$$F_{2^n} \equiv (F_{2^r} \otimes I_{2^s}) T_{2^s}^{2^r 2^s} (I_{2^r} \otimes F_{2^r}) L_{2^r}^{2^r 2^s}$$

- Two degrees of freedom: r and s
- Constraint: $n = r + s \wedge r \neq n \wedge s \neq n$
- Parameterized right-hand-side on r, s , and proof that constraint is satisfied
- Proof of equivalence for all such constrained r and s .
- A way to generate pairs (r, s)
- Proof that any such pair satisfies constraint
- Proof that all such pairs are generated

Formal Verification Effort

```
Program Definition cooley_tukey_rule n : rule F_{n} :=
{| r_dof := 2
; r_constraint := (fun (r s : nat) => r+s = n ∧ r ≠ n ∧ s ≠ n)
; r_rhs := (fun r s (H : _) =>
              (((F_{r} ⊗ I_{s})
                × T_{r, s}
                × (I_{r} ⊗ F_{s})
                × L_{r, s}) : { (proj1 H) }))
; r_gen := sum_gen n (* list (nat*nat) *)
|}.
```

Next Obligation.

```
(* Proving r_correct : rule_correct _ r_constraint
   i.e.  $\forall r s (H : r\_constraint\ r\ s),$ 
    $F_{\{n\}} \equiv r\_rhs\ r\ s\ H$  *)
```

...

Defined.

Algorithm Generation

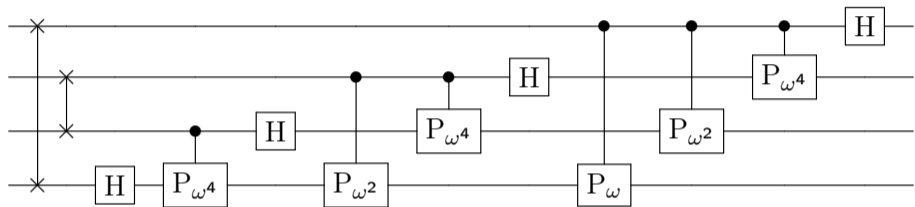
- Fueled search for all algorithms
- Single Step
 - Applying a rule to an applicable sub-expressions produces a list of results
 - Recursively rewrite subexpressions and concatenate results
- Parameterized rewrite rules produce alternative algorithms
- Fuel needed is roughly the number of qubits plus a small constant

Coq Development metrics

- 9167 loc
- 112 Definitions, mostly non-recursive
- 541 lemmas
- Roughly half of the actual proving dedicated to digit-permutations and additional supporting linear algebra

Alternative Algorithms

Example breakdown: 4-qubit QFT using the iterative radix-2 factorization



QFT_{16}






$$\begin{aligned} &= (\text{H} \otimes \text{I}_8)(\text{C}(\text{P}_{\omega^4} \otimes \text{I}_4))(\text{C}(\text{I}_2 \otimes \text{P}_{\omega^2} \otimes \text{I}_2))(\text{C}(\text{I}_4 \otimes \text{P}_{\omega})) \\ &\times (\text{I}_2 \otimes \text{H} \otimes \text{I}_4)(\text{I}_2 \otimes \text{C}(\text{P}_{\omega^4} \otimes \text{I}_2))(\text{I}_2 \otimes \text{C}(\text{I}_2 \otimes \text{P}_{\omega^2})) \\ &\times (\text{I}_4 \otimes \text{H} \otimes \text{I}_2)(\text{I}_4 \otimes \text{C}\text{P}_{\omega^4}) \\ &\times (\text{I}_8 \otimes \text{H})(\text{I}_2 \otimes \text{SWAP} \otimes \text{I}_2)\text{SWAP}_{0,3} \end{aligned}$$

Summary

- Formally verified (in Coq)...
 - derivation of quantum algorithms (SPL)
 - and the resulting circuits (SQIR)
 - using matrix semantics
- Generated alternative algorithms for future exploration and optimization

Future Work

- Gate optimization
- Quantum Measurements
- Additional Quantum Algorithms

-  *The Coq proof assistant reference manual*. The Coq development team. 2022.
-  “A Verified Optimizer for Quantum Circuits”. Kesha Hietala et al. 2021.
-  *QuantumLib*. QWIRE Team. 2022.
-  “SPIRAL: Extreme Performance Portability”. F. Franchetti et al. 2018.
-  *Optimized Quantum Circuit Generation with SPIRAL*. Scott Mionis. 2021.