BERKELEY LAB
Bringing Science Solutions to the World

U.S. DEPARTMENT OF ENERGY

Quantum Circuit Synthesis

Roel Van Beeumen

rvanbeeumen@lbl.gov

www.roelvanbeeumen.be

CSSS Talk
June 16, 2020

Outline

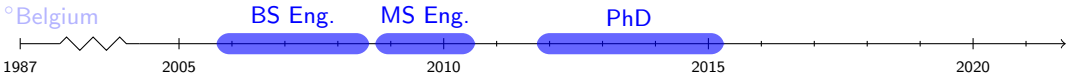
1. From Eigenvalues to Quantum Computing
2. Qubits and Quantum Circuits
3. Quantum Fourier Transform

°Belgium

1987 2005 2010 2015 2020

Belgium

- Capital: Brussels
- Population: 11,000,000
- King: Filip I



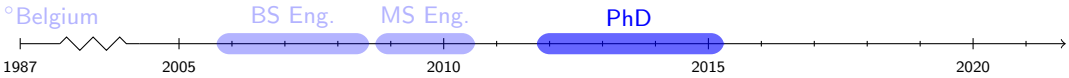
STEM Career:

- 2005–2008: **BS** Mechanical-Electrical Engineering
- 2008–2010: **MS** Mathematical Engineering
- 2011–2015: **PhD** Computer Science

KU Leuven, University of Leuven, Belgium

KU Leuven, University of Leuven

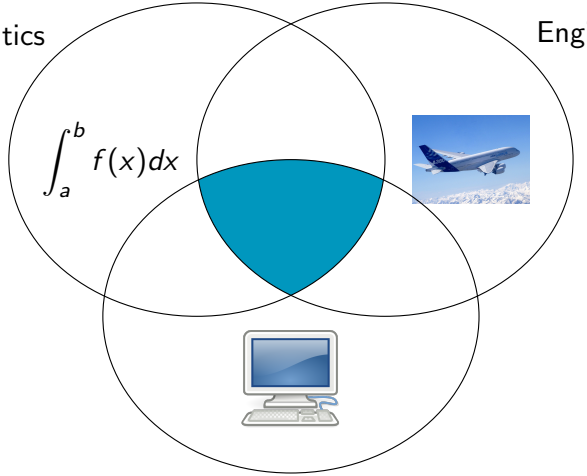
- Founded: 1425
- Students: 50,000
- Tuition: $1,000



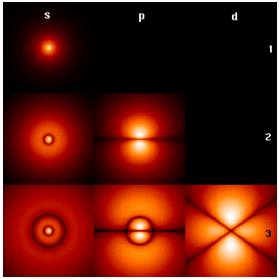
PhD Thesis:

Rational Krylov methods for nonlinear eigenvalue problems

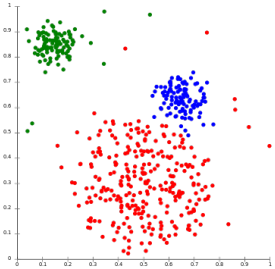
My Research

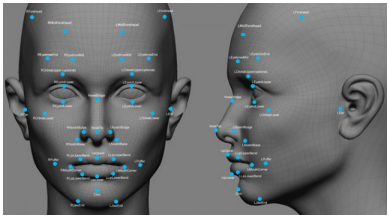


Eigenvalue problems

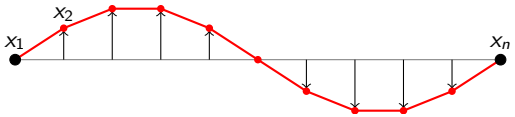


Eigenvalue problems





Linear eigenvalue problem



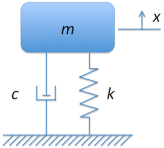
The eigenvalues and eigenmodes of a string are the solution of

$$\underbrace{\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}}_{x} = \lambda \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}}_{x}$$

where

- λ is an eigenvalue
- x is an eigenvector

Quadratic eigenvalue problem



Vibration analysis in structural analysis gives rise to

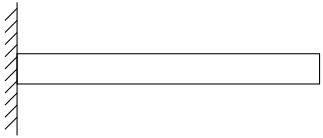
$$(\lambda^2 M + \lambda C + K)x = 0$$

where

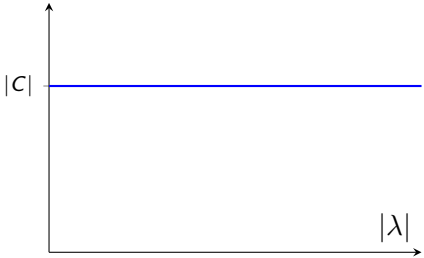
- λ is an eigenvalue
- x is an eigenvector
- M is the mass matrix
- C is the damping matrix
- K is the stiffness matrix

Nonlinear damping

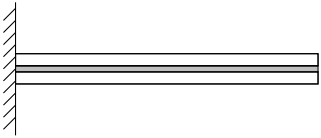
Clamped beam:



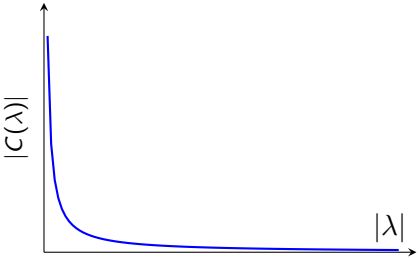
$$\left(\lambda^2 M + \lambda C + K\right) x = 0$$



Clamped sandwich beam:



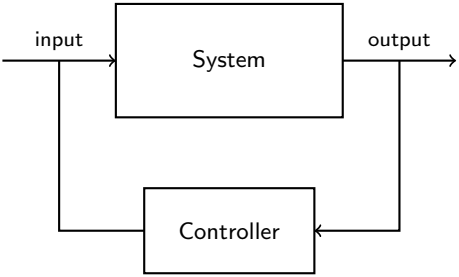
$$\left(\lambda^2 M + C(\lambda) + K\right) x = 0$$



for λ on the imaginary axis

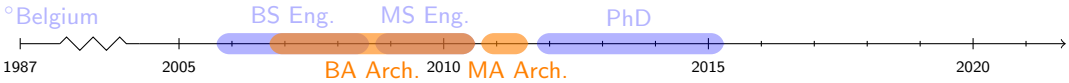
Active damping

Active damping in cars:



Delay eigenvalue problem

$$\left(\lambda^2 M + \lambda C + K + e^{-\lambda\tau} E\right) x = 0$$



STEM Career:

- 2005–2008: **BS** Mechanical-Electrical Engineering

  2006–2010: **BA** Archaeology

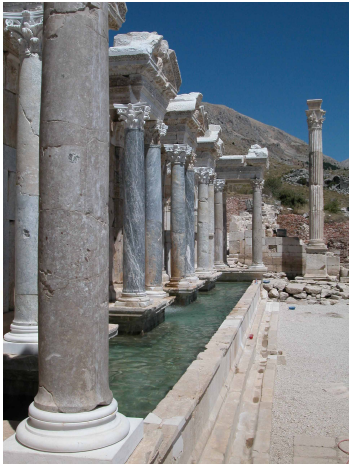
- 2008–2010: **MS** Mathematical Engineering

  2010–2011: **MA** Archaeology

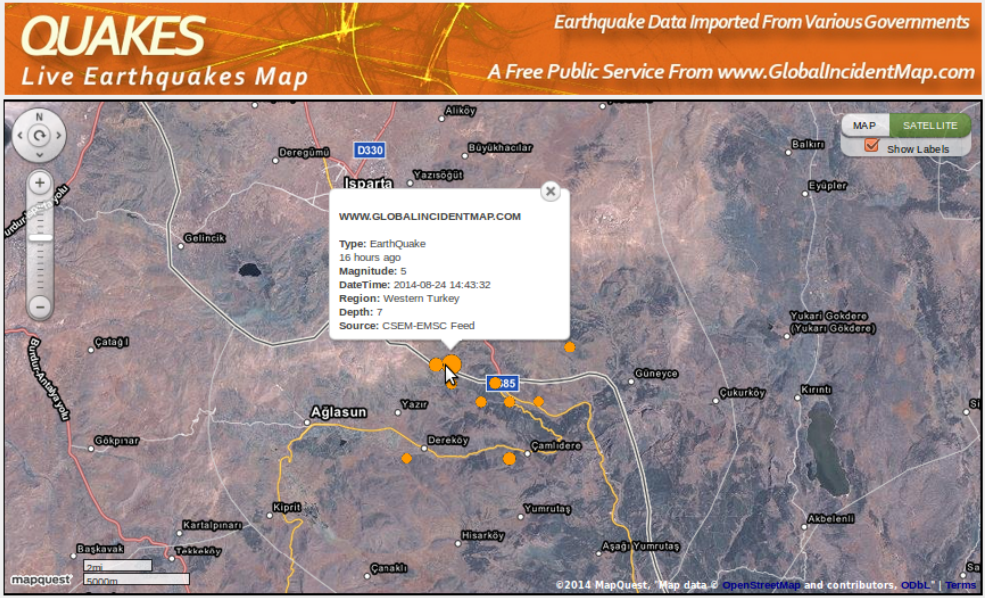
- 2011–2015: **PhD** Computer Science

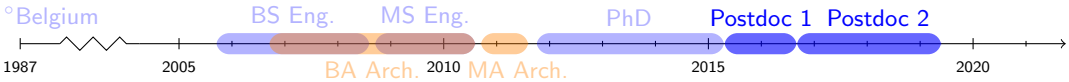
KU Leuven, University of Leuven, Belgium

Sagalassos Archaeological Research Project (Turkey)



Sagalassos Archaeological Research Project (Turkey)





STEM Career:

- 2005–2008: **BS** Mechanical-Electrical Engineering

  2006–2010: **BA** Archaeology

- 2008–2010: **MS** Mathematical Engineering

  2010–2011: **MA** Archaeology

- 2011–2015: **PhD** Computer Science

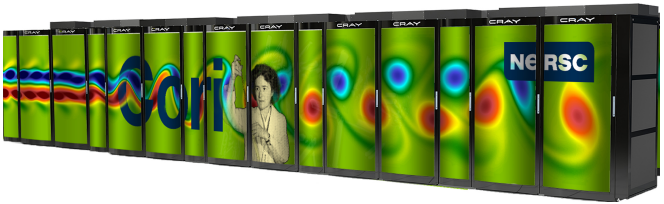
- 2015–2016: **Postdoc** @ KU Leuven

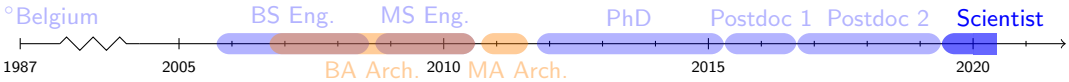
- 2016–2019: **Postdoc** @ Berkeley Lab

Postdoc @ Berkeley Lab

- LBNL Postdoc:
  → Computing Sciences Area
  → Computational Research Division
  → Applied Mathematics Department
  → Scalable Solvers Group

- Research Projects:
  - Eigenvalue problems
  - Model order reduction
  - Numerical software development

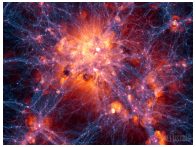


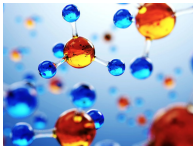


- Since 2019: Career-track **Research Scientist** @ Berkeley Lab
- 2019 LDRD Early Career Award
  - Project: *Approximate Unitary Matrix Decompositions for Quantum Circuit Synthesis*
  - 1st Postdoc: Daan Camps

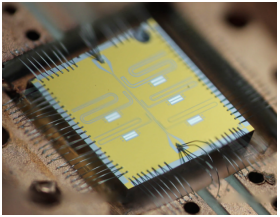
Compiling Quantum Programs: Quantum Circuit Synthesis

Quantum Applications

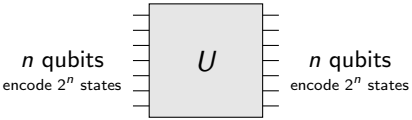




Quantum Chip



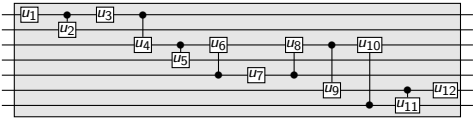
Quantum Program



a quantum program U, is a unitary matrix of size $2^n \times 2^n$, too large to write down for large n

$\longrightarrow$

Quantum Circuit



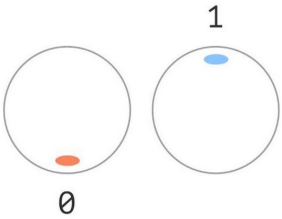
is a series of quantum gates, each performing a simple unitary transformation on only a few qubits

Qubits and Quantum Circuits

Classical Bit versus Qubit

Classical bit

2 states: 0 and 1



Quantum bit

linear combinations: $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

Computational basis states

$$|0\rangle := \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |1\rangle := \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad |\alpha|^2 + |\beta|^2 = 1$$

Kronecker Products

Kronecker product of matrices A and B

$$A \otimes B := \begin{bmatrix} a_{11}B & a_{12}B & \cdots & a_{1,m}B \\ a_{21}B & a_{22}B & \cdots & a_{2,m}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{n,1}B & a_{n,2}B & \cdots & a_{n,m}B \end{bmatrix}$$

Properties

$$(\gamma A) \otimes B = A \otimes (\gamma B) = \gamma(A \otimes B)$$

$$A \otimes (B + C) = A \otimes B + A \otimes C$$

$$(B + C) \otimes A = B \otimes A + C \otimes A$$

and

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$$

Unit Vectors and Identity Matrix

Unit vectors

$$e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle \qquad e_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle$$

Identity matrix

$$I_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}}_{E_1 = e_1 e_1^\top} + \underbrace{\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}}_{E_2 = e_2 e_2^\top}$$

Direct sum

$$A \oplus B = \begin{bmatrix} A & \\ & B \end{bmatrix} = E_1 \otimes A + E_2 \otimes B$$

Multiple qubits

2 qubits:

$$|\psi\rangle = \alpha\,|00\rangle + \beta\,|01\rangle + \gamma\,|10\rangle + \delta\,|11\rangle$$

$$|00\rangle := \begin{bmatrix}1\\0\\0\\0\end{bmatrix} \qquad |01\rangle := \begin{bmatrix}0\\1\\0\\0\end{bmatrix} \qquad |10\rangle := \begin{bmatrix}0\\0\\1\\0\end{bmatrix} \qquad |11\rangle := \begin{bmatrix}0\\0\\0\\1\end{bmatrix} \qquad |\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1$$

n qubits:

- state space of dimension 2^n
- linear combination of 2^n computational basis states

$$|\psi\rangle = \sum_{\mathtt{j}_1,\ldots,\mathtt{j}_n=1}^{2} \alpha_{\mathtt{j}_1\mathtt{j}_2\cdots\mathtt{j}_n} \left(e_{\mathtt{j}_1} \otimes e_{\mathtt{j}_2} \otimes \cdots \otimes e_{\mathtt{j}_n}\right)$$

Quantum Circuits

Matrix notation

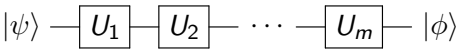
$$\phi = U\psi$$

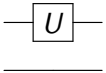
$$\phi = U_m \cdots U_2 U_1 \psi$$

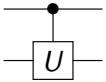
$$U \otimes I$$

$$U_{\text{ctr}} = I \oplus U = \begin{bmatrix} I & \\ & U \end{bmatrix}$$

Quantum circuit







Quantum Gates

Hadamard $\quad -\boxed{H}- \quad \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$

Phase $\quad -\boxed{S}- \quad \begin{bmatrix}1 & 0\\ 0 & \mathrm{i}\end{bmatrix}$

$\pi/8$ $\quad -\boxed{T}- \quad \begin{bmatrix}1 & 0\\ 0 & e^{\mathrm{i}\pi/4}\end{bmatrix}$

Pauli-X $\quad -\boxed{X}- \quad \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$

Pauli-Y $\quad -\boxed{Y}- \quad \begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix}$

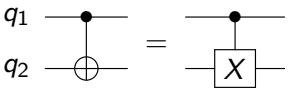
Pauli-Z $\quad -\boxed{Z}- \quad \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$

Controlled-NOT (CNOT)

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

CNOT gate: definition

- 1st qubit q_1: control
- 2nd qubit q_2: target



- controlled operation:

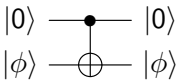
$$U_{\text{ctr}} = I \oplus X = E_1 \otimes I + E_2 \otimes X$$

- controlled NOT:

$$\text{CNOT} = \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}}_{E_1} \otimes \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}_{I} + \underbrace{\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}}_{E_2} \otimes \underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}_{X} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{bmatrix}$$

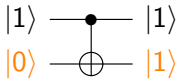
CNOT gate: behavior

target bit $= |0\rangle$



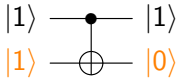
$$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{bmatrix} \begin{bmatrix} * \\ * \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} * \\ * \\ 0 \\ 0 \end{bmatrix} = |0\phi\rangle$$

target bit $= |1\rangle$



$$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = |11\rangle$$

$$|00\rangle := \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad |01\rangle := \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

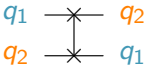


$$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = |10\rangle$$

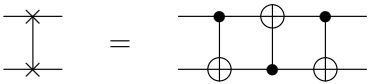
$$|10\rangle := \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \qquad |11\rangle := \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

SWAP gate: implemented by 3 CNOTs

SWAP gate:



can be implemented by 3 CNOTs



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

$$|00\rangle := \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad |01\rangle := \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \qquad |10\rangle := \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \qquad |11\rangle := \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Quantum Fourier Transform

Discrete Fourier Transform (DFT)

x: vector of length N $\longrightarrow$ y: vector of length N

$$y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \omega_N^{kj} x_j, \qquad \text{with} \qquad \omega_N := e^{\frac{-2\pi \mathrm{i}}{N}}$$

Matrix notation

$$y = F_N x, \qquad F_N := \frac{1}{\sqrt{N}} \begin{bmatrix} \omega_N^0 & \omega_N^0 & \omega_N^0 & \cdots & \omega_N^0 \\ \omega_N^0 & \omega_N^1 & \omega_N^2 & \cdots & \omega_N^{N-1} \\ \omega_N^0 & \omega_N^2 & \omega_N^4 & \cdots & \omega_N^{2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \omega_N^0 & \omega_N^{N-1} & \omega_N^{2(N-1)} & \cdots & \omega_N^{(N-1)(N-1)} \end{bmatrix}$$

Examples

$$F_1 = \begin{bmatrix} 1 \end{bmatrix}, \quad F_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad F_3 = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1 & 1 \\ 1 & \omega_3 & \omega_3^2 \\ 1 & \omega_3^2 & \omega_3 \end{bmatrix}, \quad F_4 = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -\mathrm{i} & -1 & \mathrm{i} \\ 1 & -1 & 1 & -1 \\ 1 & \mathrm{i} & -1 & -\mathrm{i} \end{bmatrix}$$

Complexity

Matvec: $\mathcal{O}(N^2)$ $\longrightarrow$ FFT: $\mathcal{O}(N \log(N))$ $\longrightarrow$ QFT: $\mathcal{O}((\log(N)^2)$

Fast Fourier Transform (FFT)

- applies Discrete Fourier Transform in $\mathcal{O}(N \log N)$
- by recursively using radix-2 decomposition of permuted DFT matrix ($F_N = PF'_N$)

$$F'_N = \frac{1}{\sqrt{2}} \begin{bmatrix} F'_{N/2} & F'_{N/2} \\ F'_{N/2}\Omega_{N/2} & -F'_{N/2}\Omega_{N/2} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} F'_{N/2} & \\ & F'_{N/2} \end{bmatrix} \begin{bmatrix} I_{N/2} & I_{N/2} \\ \Omega_{N/2} & -\Omega_{N/2} \end{bmatrix}$$

- let $N = 2^n$ or $n = \log_2(N)$

$$F_N = PM_1M_2 \cdots M_n$$

where

$$M_k = I_{2^{n-k}} \otimes \frac{1}{\sqrt{2}} \begin{bmatrix} I_{2^{k-1}} & I_{2^{k-1}} \\ \Omega_{2^{k-1}} & -\Omega_{2^{k-1}} \end{bmatrix}, \qquad k = 1, 2, \ldots, n$$

Quantum Fourier Transform (QFT)

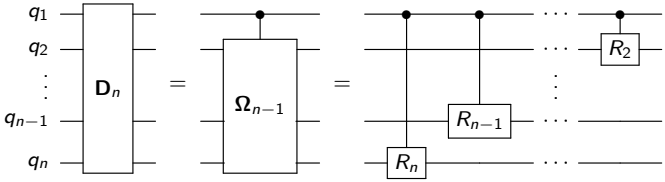
- recall the radix-2 decomposition ($F'_{2^n} = \mathbf{F}'_n$)

$$\mathbf{F}'_n = \begin{bmatrix} \mathbf{F}'_{n-1} & \\ & \mathbf{F}'_{n-1} \end{bmatrix} \begin{bmatrix} \mathbf{I}_{n-1} & \\ & \mathbf{\Omega}_{n-1} \end{bmatrix} \left(\frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{I}_{n-1} & \mathbf{I}_{n-1} \\ \mathbf{I}_{n-1} & -\mathbf{I}_{n-1} \end{bmatrix} \right)$$
$$= (I_2 \otimes \mathbf{F}'_{n-1}) \underbrace{(\mathbf{I}_{n-1} \oplus \mathbf{\Omega}_{n-1})}_{\mathbf{D}_n} (H \otimes \mathbf{I}_{n-1})$$

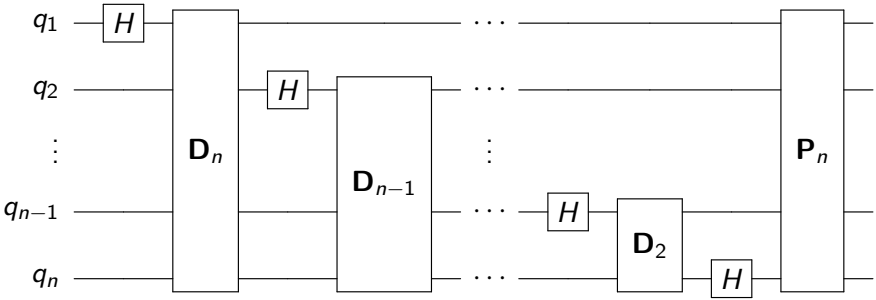
where

$$\mathbf{\Omega}_n = R_2 \otimes R_3 \otimes \cdots \otimes R_n \otimes R_{n+1}, \qquad R_k := \begin{bmatrix} 1 & \\ & \omega_{2^k} \end{bmatrix}$$

- quantum circuit for diagonal blocks



QFT Circuit



- complexity: $\mathcal{O}\big((\log(N)^2\big)$
- in matrix notation

$$\mathbf{F}_n = \mathbf{P}_n \mathbf{F}'_n = \mathbf{P}_n \mathbf{M}_1 \mathbf{M}_2 \cdots \mathbf{M}_n$$

where

$$\mathbf{M}_k = \mathbf{I}_{n-k} \otimes \left[\mathbf{D}_k (H \otimes \mathbf{I}_{k-1})\right], \qquad k = 1, 2, \ldots, n$$

Conclusions

Deriving the QFT from the FFT

- by decomposing diagonal factors in FFT decomposition
- extend radix-2 to radix-d QFT decomposition
- QFT decomposition and corresponding circuit is not unique

Reference:

- Camps, Van Beeumen, Yang. "*Quantum Fourier Transform Revisited*." arXiv:2003.03011

Acknowledgments:

- LBNL LDRD Program under U.S. Department of Energy Contract No. DE-AC02-05CH11231