QCE: A Simulator for Quantum Computer Hardware

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Contents

Introduction

- Simulation is an integral part of the design process of each new generation of microprocessors
- Simulate physical model representing the hardware implementation of a quantum processor may prove essential
- Conventional digital circuits: Internal working of each basic unit is irrelevant for the logical operation of the whole machine
- QC: Internal quantum dynamics of each elementary unit is a key ingredient of the QC itself

It is essential to incorporate into a simulation model the physics of the elementary units that make up the QC

Qubit

- One qubit ≡ one spin-1/2 system ≡ two-state quantum system

$$\left|\uparrow\right\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv \left|0\right\rangle$$

$$\left|\downarrow\right\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv \left|1\right\rangle$$

Basis states spanning the Hilbert spacce

- Qubit:

$$\boldsymbol{\alpha}\left|0\right\rangle + \boldsymbol{\beta}\left|1\right\rangle \quad ; \quad \boldsymbol{\alpha}, \boldsymbol{\beta} \in \boldsymbol{C}$$

BUT measurement always gives $\left|0\right\rangle$ or $\left|1\right\rangle$

3-qubit quantum computer (QC)

- QC hardware can be modeled in terms of quantum spins, i.e. qubits, that evolve in time according to the time-dependent Schrödinger equation (TDSE)

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle \qquad (\hbar = 1)$$

- The state $|\psi(t)\rangle$ describes the state of the whole QC at time *t*

$$|\psi(t)\rangle = a(\downarrow,\downarrow,\downarrow;t)|\downarrow,\downarrow,\downarrow\rangle + a(\downarrow,\downarrow,\uparrow;t)|\downarrow,\downarrow,\uparrow\rangle + \ldots + a(\uparrow,\uparrow,\uparrow;t)|\uparrow,\uparrow,\uparrow\rangle$$

3-qubit quantum computer (QC)

- Time-dependent Hamiltonian: Model for a universal 3-qubit QC

$$\boldsymbol{H}(\boldsymbol{t}) = -\boldsymbol{J}_{1,2,\boldsymbol{z}}\boldsymbol{S}_1^{\boldsymbol{z}}\boldsymbol{S}_2^{\boldsymbol{z}} - \boldsymbol{J}_{1,3,\boldsymbol{z}}\boldsymbol{S}_1^{\boldsymbol{z}}\boldsymbol{S}_3^{\boldsymbol{z}} - \boldsymbol{J}_{2,3,\boldsymbol{z}}\boldsymbol{S}_2^{\boldsymbol{z}}\boldsymbol{S}_3^{\boldsymbol{z}}$$

$$-\sum_{\boldsymbol{j}=1}^{3}\sum_{\boldsymbol{\alpha}=\boldsymbol{x},\boldsymbol{y},\boldsymbol{z}}\boldsymbol{h}_{\boldsymbol{j},\boldsymbol{\alpha},0}\boldsymbol{S}_{\boldsymbol{j}}^{\boldsymbol{\alpha}}$$

$$-\sum_{\boldsymbol{j}=1}^{3}\sum_{\boldsymbol{\alpha}=\boldsymbol{x},\boldsymbol{y},\boldsymbol{z}}\boldsymbol{h}_{\boldsymbol{j},\boldsymbol{\alpha},1}\sin\left(\boldsymbol{f}_{\boldsymbol{j},\boldsymbol{\alpha}}\boldsymbol{t}+\boldsymbol{\varphi}_{\boldsymbol{j},\boldsymbol{\alpha}}\right)\boldsymbol{S}_{\boldsymbol{j}}^{\boldsymbol{\alpha}}$$

$\boldsymbol{S}_{\boldsymbol{j}}^{\boldsymbol{\alpha}}$: $\boldsymbol{\alpha}$ - th component of the spin-1/2 operator representing qubit $\boldsymbol{j}$

$\boldsymbol{J}_{\boldsymbol{j},\boldsymbol{k}}$: strength of interaction between qubits $\boldsymbol{j}$ and $\boldsymbol{k}$

$\boldsymbol{h}_{\boldsymbol{j},\boldsymbol{\alpha},0}$: static (magnetic) field acting on qubit $\boldsymbol{j}$

$\boldsymbol{h}_{\boldsymbol{j},\boldsymbol{\alpha},1}$: periodic (RF) field acting on qubit $\boldsymbol{j}$

$\boldsymbol{f}_{\boldsymbol{j},\boldsymbol{\alpha}}$: frequency of RF field

$\boldsymbol{\varphi}_{\boldsymbol{j},\boldsymbol{\alpha}}$: phase of RF field

Quantum algorithm (QA)

- A QA consists of a sequence of micro instructions (MI) that change the state $\left|\Psi(t)\right\rangle$ of the quantum processor according to the TDSE, i.e. by a product of unitary transformations.
- Action of a MI on $\left|\Psi(t)\right\rangle$: Specification of
  - Time interval τ during which the MI is active
  - All the *J* and *h* appearing in *H(t)*, *J* and *h* are fixed during the operation of the MI

$$\Psi(t) \xrightarrow{\text{MI}} \Psi(t+\tau)$$

INPUT **OUTPUT**

Single bit operations

- Three components of spin-1/2 operator $\vec{S}$ acting on the Hilbert space spanned by $|0\rangle$ and $|1\rangle$

$$S^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \; S^y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \; S^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\hbar = 1)$$

- Rotations of spin *j* about $\pi/2$ around the *x*- and *y*-axis

$$X_j \equiv e^{i\pi S_j^x/2} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$$

$$Y_j \equiv e^{i\pi S_j^y/2} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

Single bit operations

$$\boldsymbol{X}_1 \begin{pmatrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{pmatrix} \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & \boldsymbol{i} & 0 \\ 0 & 1 & 0 & \boldsymbol{i} \\ \boldsymbol{i} & 0 & 1 & 0 \\ 0 & \boldsymbol{i} & 0 & 1 \end{pmatrix} \begin{pmatrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{pmatrix}$$

$$\boldsymbol{X}_1 |11\rangle = \left(|11\rangle + \boldsymbol{i}|01\rangle\right)/\sqrt{2}$$
$$\bar{\boldsymbol{X}}_1 |11\rangle = \left(|11\rangle - \boldsymbol{i}|01\rangle\right)/\sqrt{2}$$

$$\boldsymbol{Y}_2 \begin{pmatrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{pmatrix} \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{pmatrix}$$

$$\boldsymbol{Y}_2 |11\rangle = \left(|11\rangle + |10\rangle\right)/\sqrt{2}$$
$$\bar{\boldsymbol{Y}}_2 |11\rangle = \left(|11\rangle - |10\rangle\right)/\sqrt{2}$$

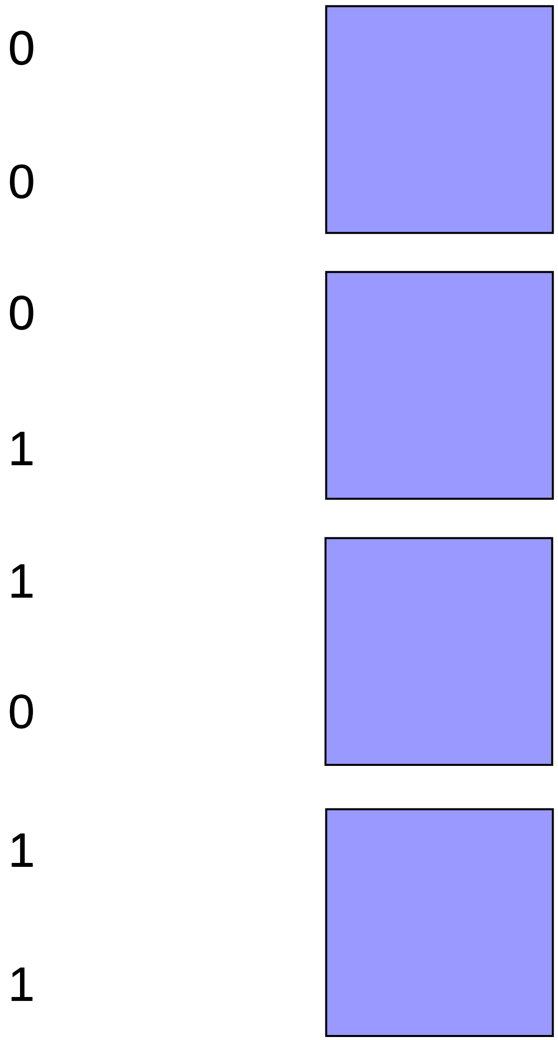
Communication

NO computation without communication

- Two qubits *j* and *k* communicate with each other through the interaction-controlled phase shift

$$I_{jk} = \begin{pmatrix} e^{i\phi_{00}} & 0 & 0 & 0 \\ 0 & e^{i\phi_{10}} & 0 & 0 \\ 0 & 0 & e^{i\phi_{01}} & 0 \\ 0 & 0 & 0 & e^{i\phi_{11}} \end{pmatrix}$$

CNOT gate



Input (IN) and output (OUT) states for the CNOT-gate

IN	OUT
$\|00\rangle$	$\|00\rangle$
$\|01\rangle$	$\|01\rangle$
$\|10\rangle$	$\|11\rangle$
$\|11\rangle$	$\|10\rangle$

CNOT gate

$$\boldsymbol{CNOT}\begin{pmatrix}|00\rangle\\|01\rangle\\|10\rangle\\|11\rangle\end{pmatrix}\equiv\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}\begin{pmatrix}|00\rangle\\|01\rangle\\|10\rangle\\|11\rangle\end{pmatrix}$$

$$\boldsymbol{CNOT}=\begin{pmatrix}\boldsymbol{I}_1&0\\0&2\boldsymbol{S}_2^x\end{pmatrix}=\begin{pmatrix}\boldsymbol{I}_1&0\\0&2\overline{\boldsymbol{Y}}_2\boldsymbol{S}_2^z\boldsymbol{Y}_2\end{pmatrix}$$

$$=\overline{\boldsymbol{Y}}_2\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&-1\end{pmatrix}\boldsymbol{Y}_2=\boldsymbol{e}^{-i\alpha}\overline{\boldsymbol{Y}}_2\boldsymbol{I}_{12}\boldsymbol{Y}_2$$

CNOT gate

$$\boldsymbol{I}_{12} = \begin{pmatrix} e^{i\phi_{00}} & 0 & 0 & 0 \\ 0 & e^{i\phi_{10}} & 0 & 0 \\ 0 & 0 & e^{i\phi_{01}} & 0 \\ 0 & 0 & 0 & e^{i\phi_{11}} \end{pmatrix} = e^{i\alpha} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\Rightarrow \quad \phi_{00} = \phi_{01} = \phi_{10} = \alpha$$

$$\phi_{11} = \alpha - \pi$$

CNOT gate: Implementation on ideal QC

- Implementation of the interaction-controlled phase shift, i.e. $I_{12} = e^{-i\tau H}$ by means of the Ising model

$$H = -J S_1^z S_2^z - h\left(S_1^z + S_2^z\right)$$

	τH	$-\phi$
$\|00\rangle$	$(-J/4-h)\tau$	$-\alpha$
$\|01\rangle$	$(J/4)\tau$	$-\alpha$
$\|10\rangle$	$(J/4)\tau$	$-\alpha$
$\|11\rangle$	$(-J/4+h)\tau$	$-\alpha+\pi$

$\Rightarrow$

$$h = -J/2$$

$$J\tau = -\pi$$

CNOT gate: Implementation on ideal QC in QCE

- How to program a 3-qubit QC so that it gives the outcome of a CNOT gate operating on the $|110\rangle$ state?
  1. Initialize QC: setting each of the three qubits to $|0\rangle$ and then flip qubits 1 and 2
     1. QP000: contains MI “initialize” which brings QC in the state $|000\rangle$
     2. QP100 (QP010): contains two MIs Y_1 (Y_2) and rotates clockwise qubit 1 (2) about π around the *Y*-axis
        Choose parameters in MI Y_1 such that $-i\tau H = i\pi S_1^y/2$
        In practice this means: $h_{1,y,0}=1, \tau/2\pi=1/4$ and all other parameters zero

CNOT gate: Implementation on ideal QC in QCE

$$H(t) = -J_{1,2,z}S_1^z S_2^z - J_{1,3,z}S_1^z S_3^z - J_{2,3,z}S_2^z S_3^z$$

$$-\sum_{j=1}^{3}\sum_{\alpha=x,y,z} h_{j,\alpha,0} S_j^\alpha$$

$$-\sum_{j=1}^{3}\sum_{\alpha=x,y,z} h_{j,\alpha,1} \sin\left(f_{j,\alpha} t + \varphi_{j,\alpha}\right) S_j^\alpha$$

CNOT gate: Implementation on ideal QC in QCE

2. Implement CNOT gate
   1. Apply MI Y_2, bringing the QC in the state $\left(|100\rangle + |110\rangle\right)/\sqrt{2}$
   2. Construct MI I_{12} with parameters $J_{1,2,z} = -1, h_{1,z,0} = h_{2,z,0} = 1/2,$ $\tau/2\pi = 1/2$ and all other parameters zero
      This brings the QC in the state $\left(|100\rangle - |110\rangle\right)/\sqrt{2}$
   3. Apply MI $-Y_2$ bringing the QC in the state $|100\rangle$
3. Expectation values of the three qubit components:

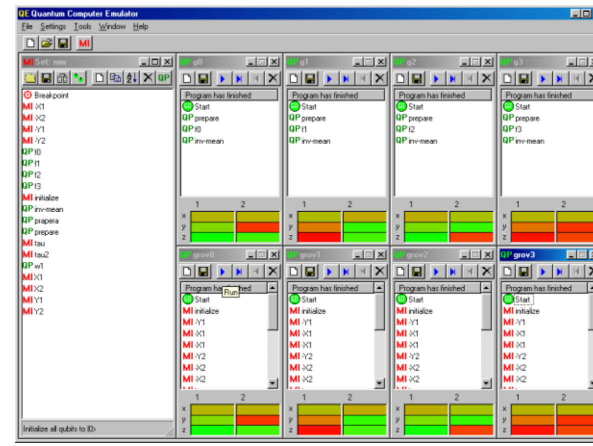
$$Q_1^x = Q_1^y = 0.5, Q_1^z = 1$$

$$Q_2^x = Q_2^y = 0.5, Q_2^z = 0$$

$$Q_3^x = Q_3^y = 0.5, Q_3^z = 0$$

Quantum Computer Emulator

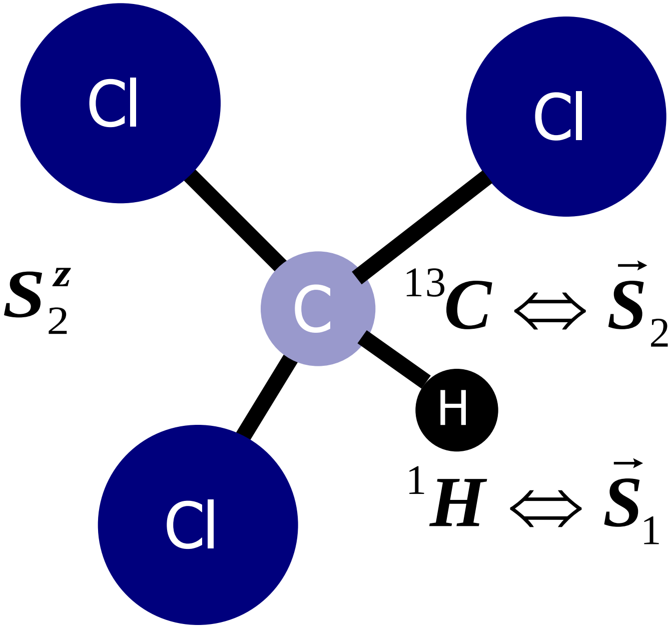
QCE



Software for Windows 98/NT4/2000/XP(SP1) download from:
http://www.compphys.org/qce.htm

CNOT gate: Implementation on a NMR-QC

- 2-qubit NMR-QC:
  Nuclear spins of carbon-13 labelled chloroform:
  - Chuang et al. (1998)



$^{13}C \Leftrightarrow \vec{S}_2$

$^{1}H \Leftrightarrow \vec{S}_1$

$$H = -J_{1,2,z} S_1^z S_2^z - h_{1,z,0} S_1^z - h_{2,z,0} S_2^z$$

$J_{1,2,z} / 2\pi \approx -215\text{Hz}$, $h_{1,z,0} / 2\pi \approx 500\text{Mhz}$,
$h_{2,z,0} / 2\pi \approx 125\text{Mhz}$

normalization →

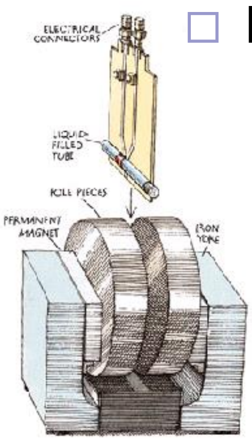
$J_{1,2,z} = -0.43 \times 10^{-6}$, $h_{1,z,0} = 1$, $h_{2,z,0} = 0.25$

$h_1 = 4h_2$

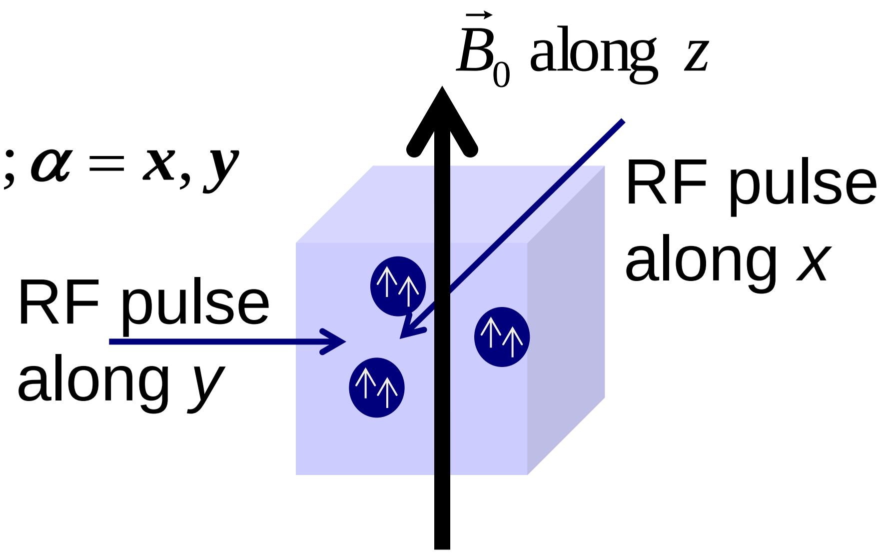
CNOT gate: Implementation on a NMR-QC

- How to perform "quantum computation" ?
  - NMR experiment

$$H^{NMR} = -J_{1,2,z} S_1^z S_2^z - h_{1,z,0} S_1^z - h_{2,z,0} S_2^z - \sum_{j=1}^{2} \sum_{\alpha=x,y} h_{j,\alpha,1} \sin\left(f_{j,\alpha} t + \varphi_{j,\alpha}\right) S_j^{\alpha}$$



  - Resonance condition
    - Address spin *j*: $f_{j,\alpha} \approx h_{j,z,0}\ ;\ \alpha = x, y$



CNOT gate: Implementation on a NMR-QC

- Application of an RF-pulse of "power" $\tau h_{j,x,1} = \pi$ has the effect of rotating spin *j* by an angle of π/2 about the *y*-axis.
- Implementation of CNOT gate:

$$H^{NMR} = H + H'$$

where

$$H = -J_{1,2,z} S_1^z S_2^z - h S_1^z - h S_2^z$$

$$H' = \left(h - h_{1,z,0}\right) S_1^z - \left(h - h_{2,z,0}\right) S_2^z$$

$$\Rightarrow \quad CNOT = e^{-i\tau\left(h_{1,z,0} - h\right) S_1^z} e^{-i\tau\left(h_{2,z,0} - h\right) S_2^x} \overline{Y}_2 e^{-i\tau H^{NMR}} Y_2$$

CNOT gate: Implementation on a NMR-QC in QCE

- How to program a 2-qubit NMR-QC so that it gives the outcome of a CNOT gate operating on the $|11\rangle$ state?
  1. Initialize QC: setting each of the two qubits to $|0\rangle$ and then flip qubits 1 and 2
     1. In all operations: $J_{1,2,z} = -0.43\times 10^{-6}$, $h_{1,z,0} = 1$, $h_{2,z,0} = 0.25$
     2. QP000: contains MI "initialize" which brings QC in the state $|00\rangle$
     3. QP100 (QP010): contains two MIs Y_1 (Y_2) and rotates clockwise qubit 1 (2) about π around the *Y*-axis
        Parameters in MI Y_1:
        1. Address spin 1: $f_{1,x} = h_{1,z,0} = f_{2,x} = 1$
        2. Rotation by an angle $\pi/2$ requires $\tau h_{1,x,1} = \pi$
           Choosing $h_{1,x,1} = 1/40$ gives $h_{2,x,1} = 1/160$ and $\tau/2\pi = 20$
        3. All other parameters are zero

        Parameters in MI Y_2: $f_{2,x} = h_{2,z,0} = f_{1,x} = 1/4, h_{2,x,1} = 1/80, h_{1,x,1} = 1/20,$

        $$\tau/2\pi = 40$$

CNOT gate: Implementation on NMR-QC in QCE

2. Implement CNOT gate

$$CNOT = e^{-i\tau(h_{1,z,0}-h)S_1^z} e^{-i\tau(h_{2,z,0}-h)S_2^x} \overline{Y}_2 e^{-i\tau H^{NMR}} Y_2$$

$$\equiv \overline{X}_1 e^{-iaS_1^y} X_1 e^{-ibS_2^x} \overline{Y}_2 e^{-i\tau H^{NMR}} Y_2$$

1. Condition CNOT: $h = -J/2, J\tau = -\pi$

$$\left(\frac{\tau}{2\pi}\right) J = -1/2 \Rightarrow \left(\frac{\tau}{2\pi}\right) = 116279.6976744186, \left(\frac{\tau}{2\pi}\right) h = 1/4$$

2. Parameters determined by molecules: $h_{1,z,0} = 1, h_{2,z,0} = 1/4$

$$a \equiv \left(\frac{\tau}{2\pi}\right)(h_{1,z,0} - h)2\pi = (1162790.4476744186)2\pi$$

$$\Rightarrow a = 0.4476744186$$

$$b \equiv \left(\frac{\tau}{2\pi}\right)(h_{2,z,0} - h)2\pi = (290697.4244186047)2\pi$$

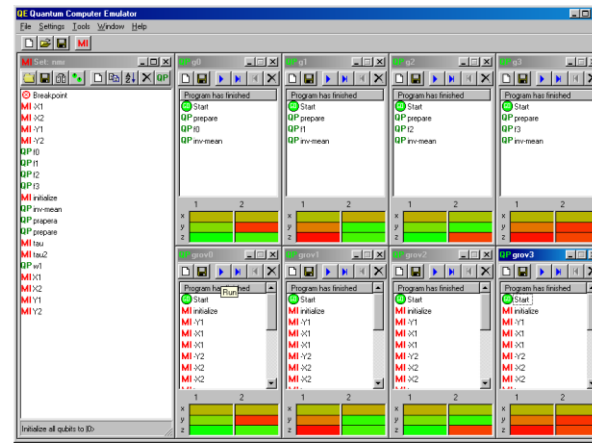
$$\Rightarrow b = 0.4244186047$$

CNOT gate: Implementation on NMR-QC in QCE

4. Apply MI Y_2
5. Construct MI H^{NMR} with parameters $J_{1,2,z} = -0.43 \times 10^{-6}$, $h_{1,z,0} = 1, h_{2,z,0} = 0.25, \tau / 2\pi = 1162790.6976744186$
6. Apply MI $-Y_2$
7. Apply MI X_{2b} with parameters
   $f_{2,y} = h_{2,z,0} = f_{1,y} = 1/4, h_{2,y,1} = 0.04244186047, h_{1,x,1} = 0.16976744188,$
   $\tau / 2\pi = 20$
8. Apply MI X_1 with parameters
   $f_{1,y} = h_{2,z,0} = f_{2,y} = 1, h_{1,y,1} = 1/40, h_{2,y,1} = -1/160,$
   $\tau / 2\pi = 20$
9. Apply MI Y_{1b} with parameters
   $f_{1,x} = h_{1,z,0} = f_{2,x} = 1, h_{1,x,1} = -0.4476744186, h_{2,x,1} = -0.11191860465,$
   $\tau / 2\pi = 20$
10. Apply MI $-X_1$

Quantum Computer Emulator

QCE



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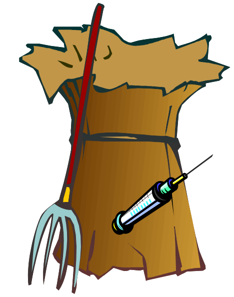
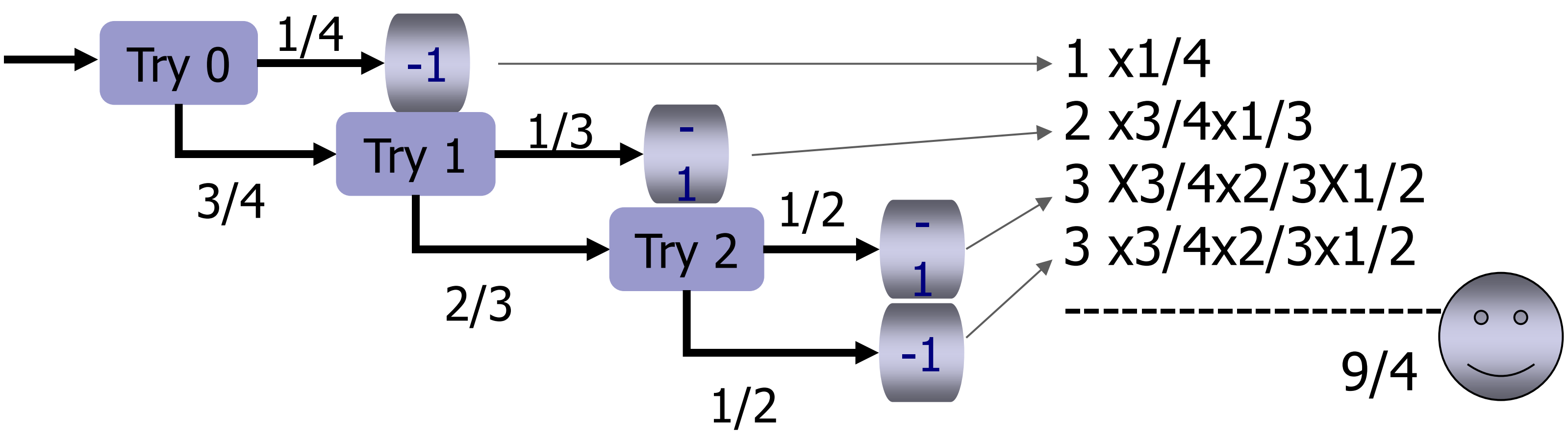
Needle in a haystack (classical version)



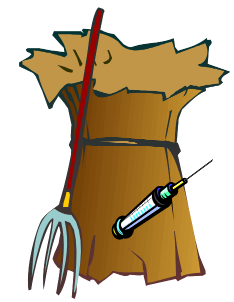
- Consider a collection of numbered items, all labelled “1” except one item which carries the label “-1”
- Example: 4 items

position	0	1	2	3
item	1	1	−1	1

  - Problem: Find the position (index) of the “-1” item
- On a “classical” computer (assuming a uniform random distribution of the “–1” item) :

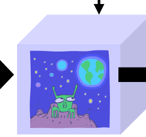


Needle in a haystack (quantum version)



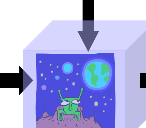
- Assume we have a magic device (the QC) that operates on linear superpositions of states
  - One "operation"

0	1	2	3
1	1	−1	1

$$|\Psi\rangle = \left(|0\rangle + |1\rangle + |2\rangle + |3\rangle\right)/2$$  $$|\Psi\rangle = \left(|0\rangle + |1\rangle - |2\rangle + |3\rangle\right)/2$$

  - L. Grover: In this case "-1" can be found in one "operation"
    - For 4 items only, in general, for *N* items : $O\left(\sqrt{N}\right)$

$$D = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{pmatrix} \quad ; \quad |\Psi\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ -1 \\ 1 \end{pmatrix} \quad \Rightarrow \quad D|\Psi\rangle = |2\rangle$$

$|\Psi\rangle$  $|2\rangle$

Needle in a Haystack: Quantum Program

Putting all pieces together …

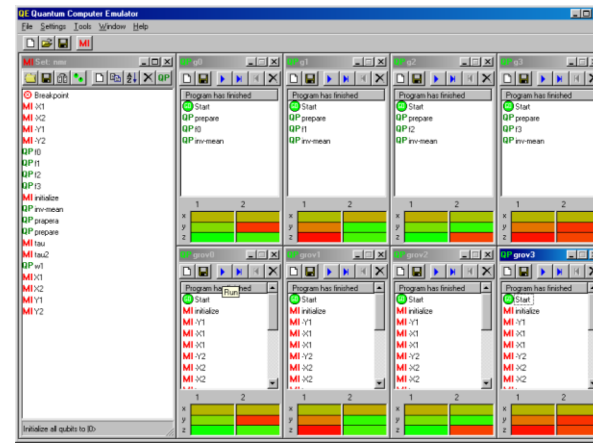
1. Prepare QC: $\bar{X}_2\bar{X}_2\bar{Y}_2\bar{X}_1\bar{X}_1\bar{Y}_1$
   - Apply pulses, reading from right to left
2. Example: "-1" item in position 2

$$P_2 = X_1\bar{Y}_1 X_2\bar{Y}_2 I(\pi)\bar{X}_1\bar{Y}_1 X_2\bar{Y}_2 I(\pi)$$

3. Read out

Quantum Computer Emulator

QCE



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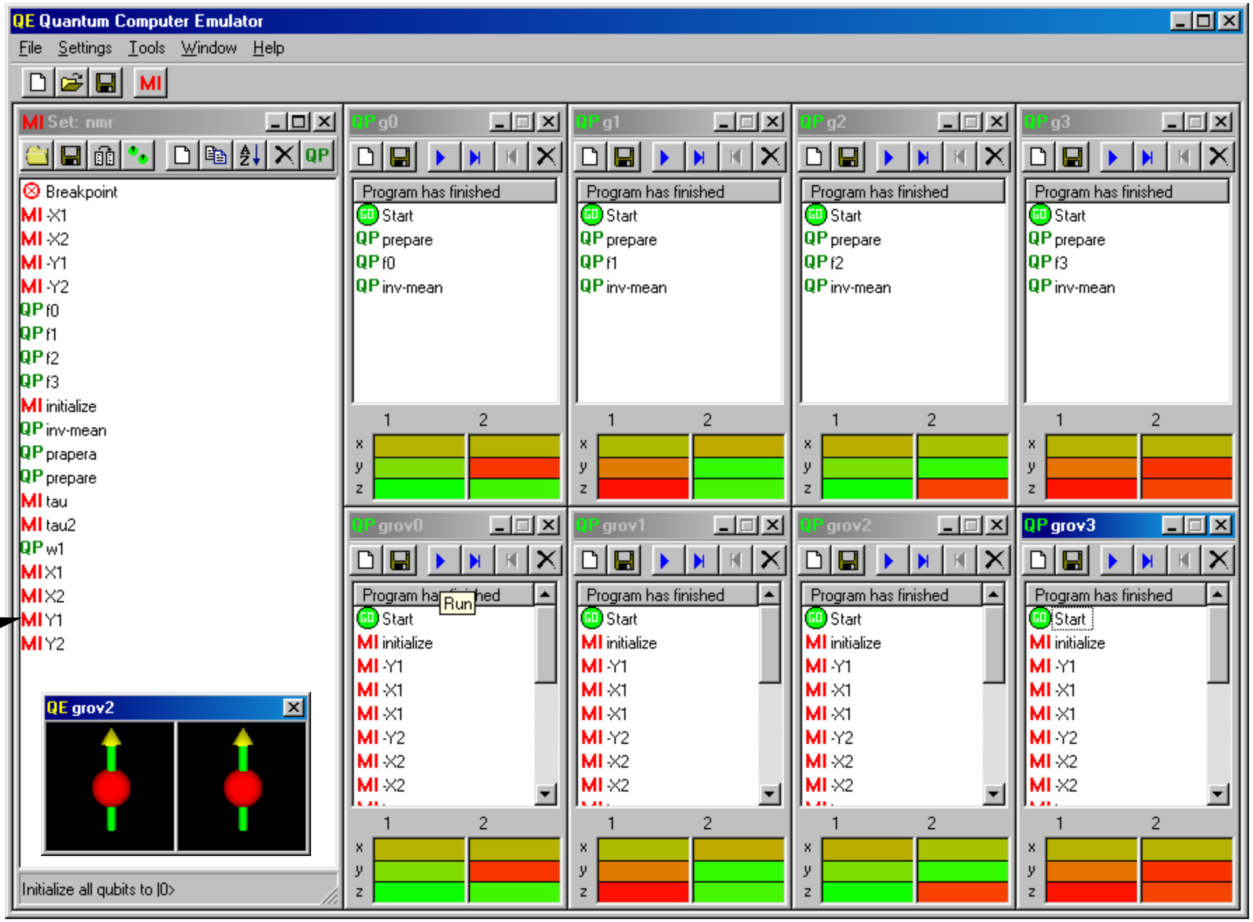
Quantum Computer Emulator (QCE)

- CNOT gate
- Toffoli gate
- QFT
- Order finding
- 3x4-qubit adder
- …

- Grover's database search algorithm
- Shor's algorithm
- Number partitioning problem
- Deutsch-Jozsa algorithm



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