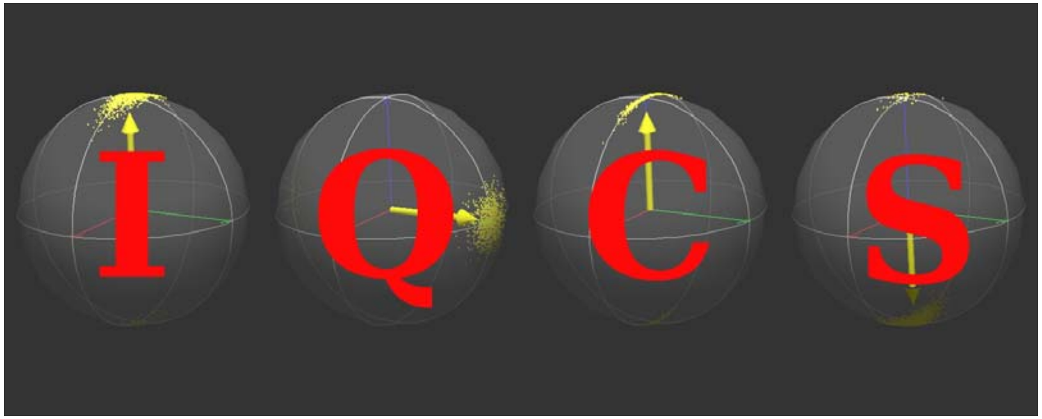
Improving Quantum Computer Simulations
DEISA project results



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Outline

- Why Quantum Computation?
- Quantum Information Basics
- Need for Simulation
- Massively Parallel QC Simulator
- DEISA: Enabling Work
- Memory Access Scheme
- Error Model
- Robustness of QFT and Grover's Algorithm
- Outlook

Why Quantum Computation?

- According to Moore's law, chips will scale down to atomic size around 2020. It is thus likely that quantum effects will become important by then.

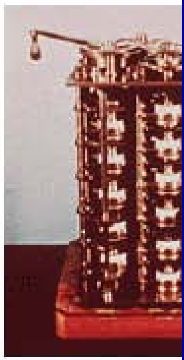
- Unitary evolution in quantum mechanics is reversible: no energy dissipation on small scale, so no limitation a priori upon computation size caused by power requirements.

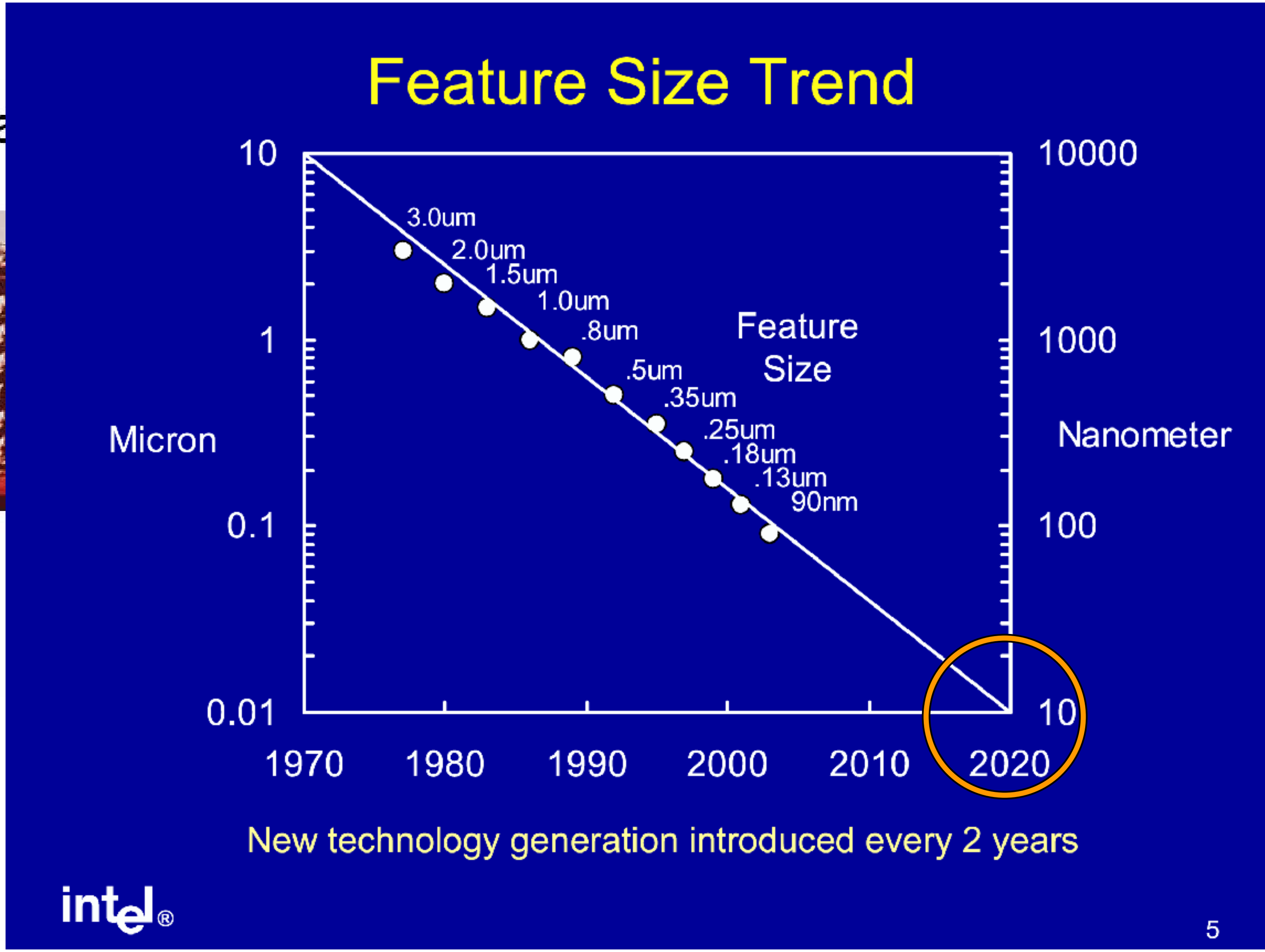
- Simulation of physical quantum systems with an exponentially large Hilbert space.

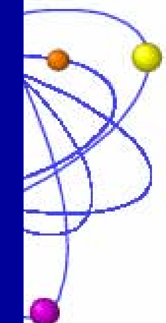
- Some computational problems could be solved by a quantum computer more efficiently than by any classical computer.

Technological Progress (Moore's Law)

faste







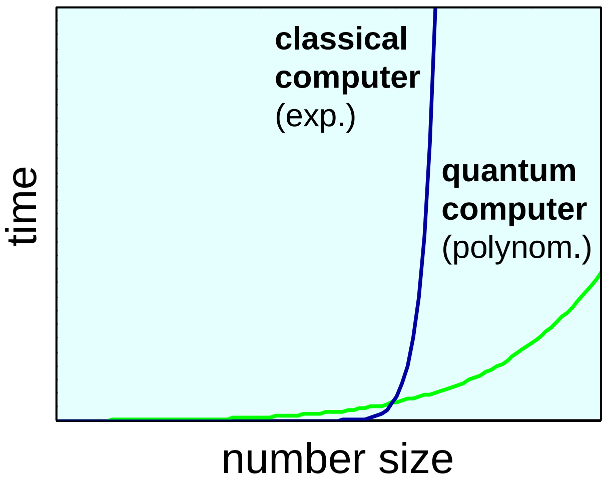
1m

Why Quantum Information Processing?

- quantum mechanical superposition states
  → massively parallel computation

- problems intractable on classical computers
  can be solved on a quantum computer

Shor '94: factorization of large numbers



Grover '96: fast searching of an unstructured data base

classical algorithm $t \propto N$

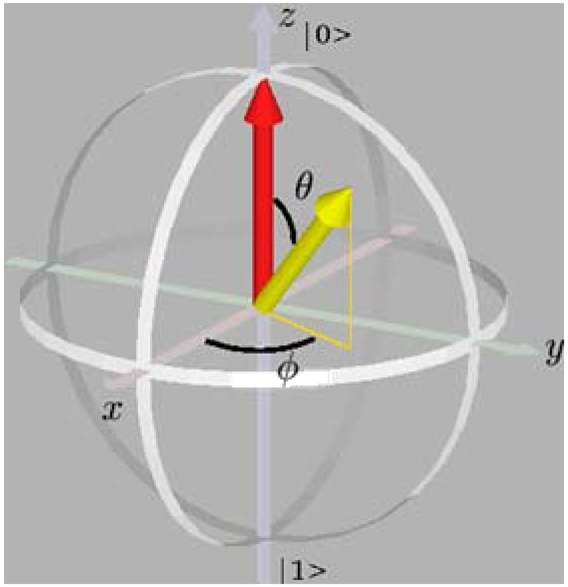
quantum algorithm $t \propto \sqrt{N}$

Classical vs. Quantum bits

Bit

0 or **1**

Qubit



$$\alpha_0 = \cos(\theta/2)$$
$$\alpha_1 = e^{i\phi}\sin(\theta/2)$$

$$|\alpha_0|^2 + |\alpha_1|^2 = 1$$

$$|\psi\rangle = \alpha_0\,|0\rangle + \alpha_1\,|1\rangle$$

State Representation

$$|0\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|1\rangle = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

1 qubit $$|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle \Longleftrightarrow \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix}$$

2 qubits $$|\psi\rangle = \alpha_{00} |00\rangle + \alpha_{01} |01\rangle + \alpha_{10} |10\rangle + \alpha_{11} |11\rangle \Longleftrightarrow \begin{pmatrix} \alpha_{00} \\ \alpha_{01} \\ \alpha_{10} \\ \alpha_{11} \end{pmatrix}$$

N qubits → 2^N dimensional state vector

Quantum Mechanical Time Evolution

- Schrödinger equation

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

- all quantum operations are unitary $U = e^{-iHt}$

$$|\psi'\rangle = U\,|\psi\rangle$$

dim U = 2^Nx2^N

- quantum computational process

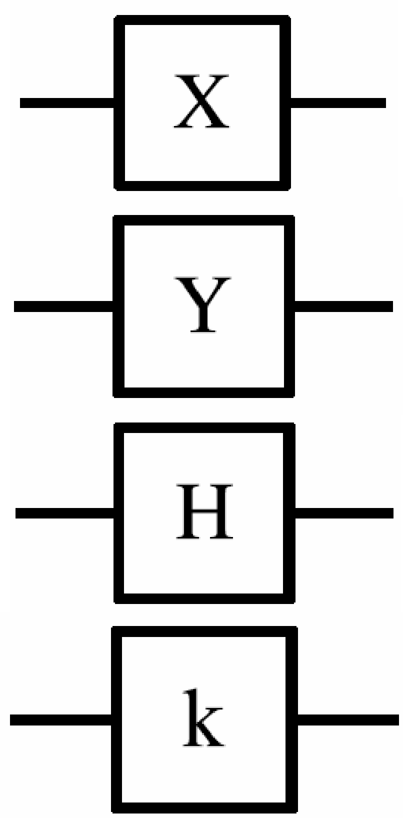
  - initialization
  - quantum operation $|\psi_{out}\rangle = U_k U_{k-1} \ldots U_1\,|\psi_{in}\rangle$
  - measurement

Universal Quantum Computer

- built of elementary One and Two-qubit operations (Phase-Shift, Hadamard, ControlledNOT) [Barenco 95]
- not unique

1-Qubit Quantum Operations

spin 1/2 operators $S^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$



X-Rotation $$X = e^{i\pi S^x/2} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$$

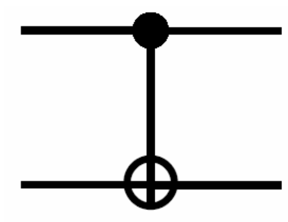
Y-Rotation $$Y = e^{i\pi S^y/2} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

Hadamard $$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

phase shift $$R(\phi) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} \qquad \phi = 2\pi/2^k$$

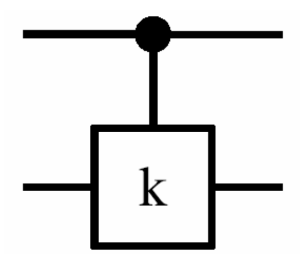
2-Qubit Quantum Operations

Controlled Not



$$C_{10} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Controlled phase shift



$$R_{10}(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix} \quad \phi = 2\pi/2^k$$

Need for Simulation

- Develop quantum algorithms
- Analyze robustness to decoherence and gate imperfections
- Test scalability of error correction codes
- Optimize steering sequences for realistic quantum computing devices

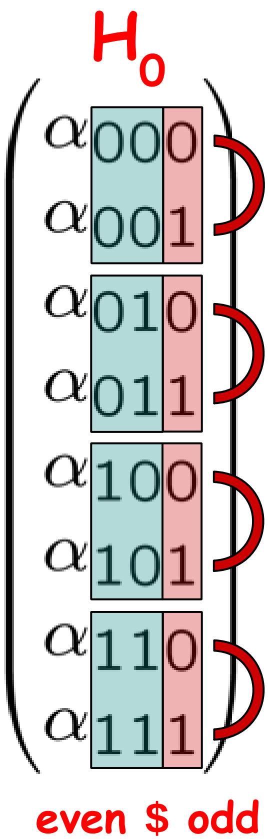
IQCS Library

- 1-, 2-, 3-qubit gate level operations
- gate imperfections / decoherence
- massively parallel (MPI / OpenMP)
- good scaling properties
- highly portable (PC(s), SMP-clusters, vector machines)

DEISA: enabling work

- no porting / adaptation needed
- 144.000 CPUh granted (comp. in Jülich)
- memory bounded problem:
  - sophisticated memory access scheme
  - inter-node communication limits performance
- job submission: UNICORE

Operations on n-qubit State Vector



$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

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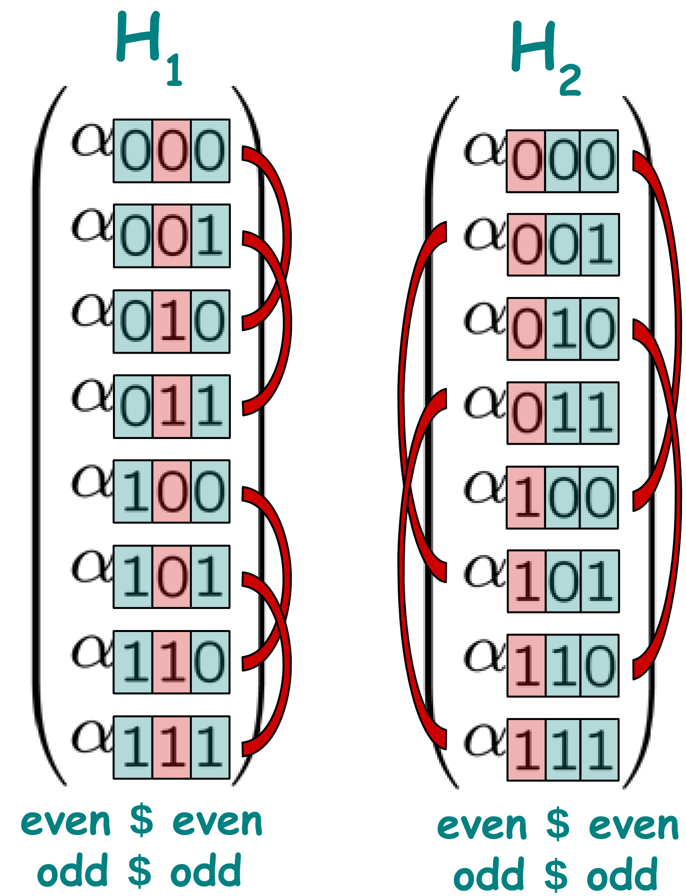
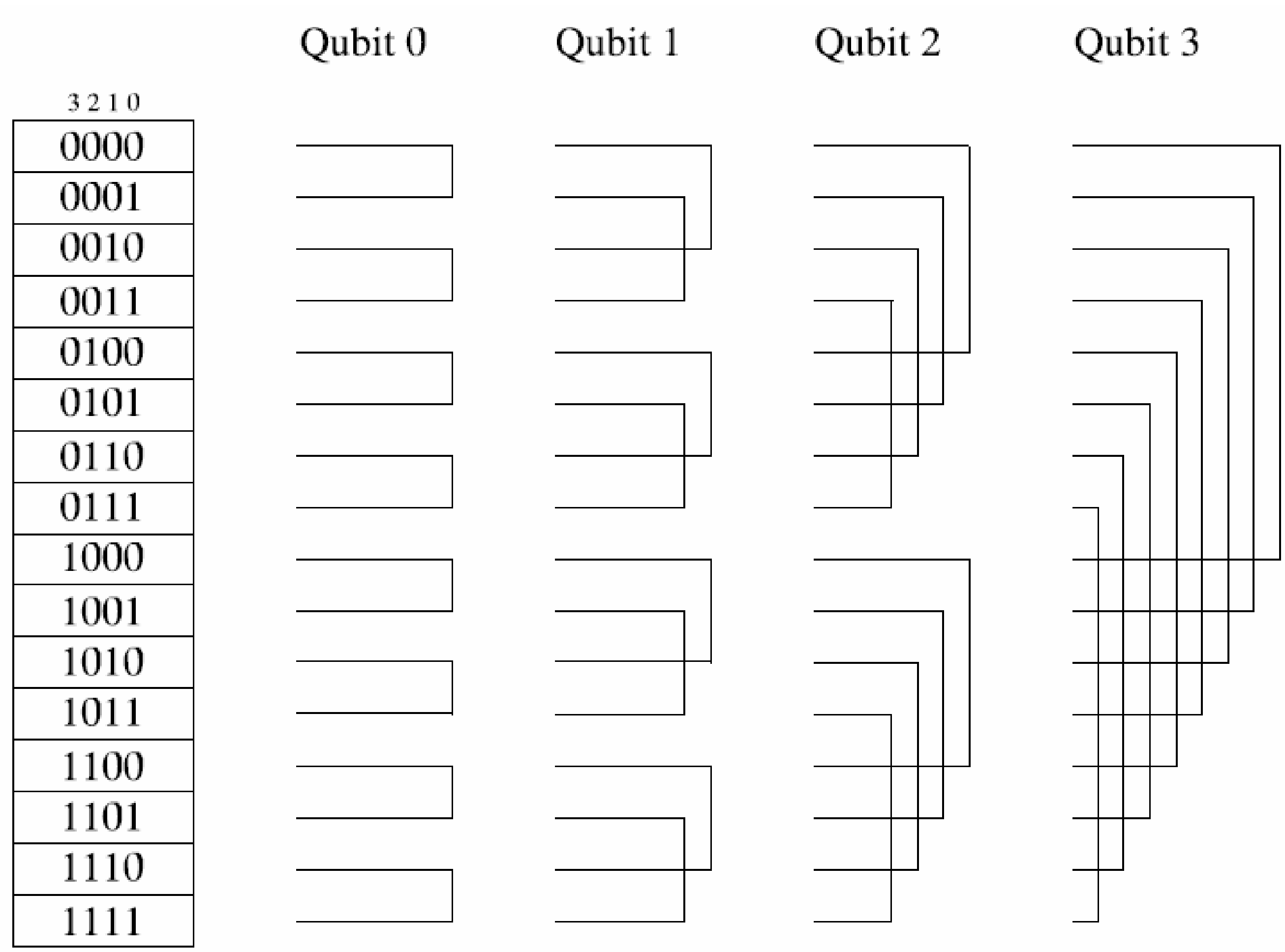
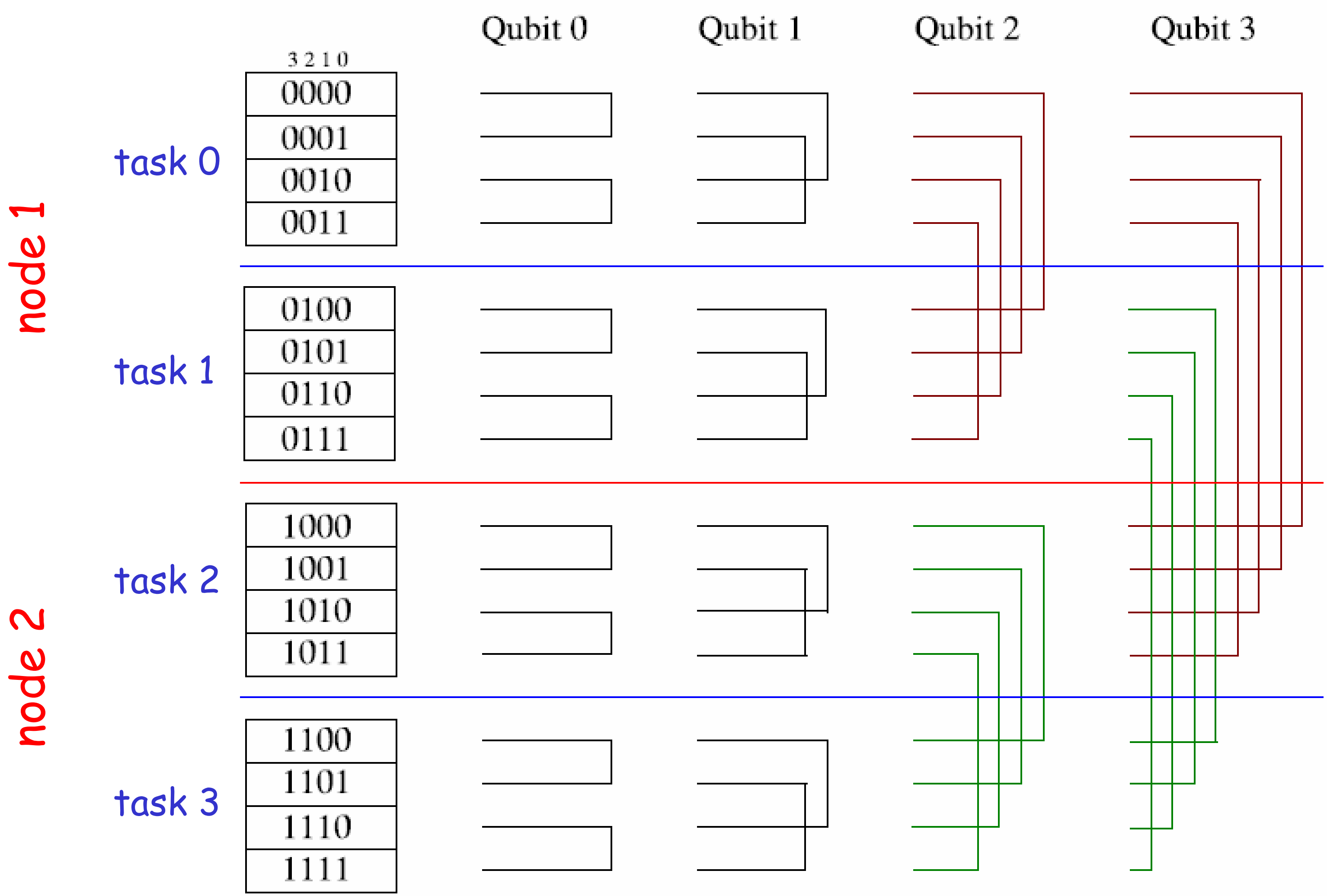


- decompose H_q into 2^{n-1} single qubit operations H
- single qubit operations H commute
- stride $|l-k|=2^q$

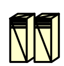
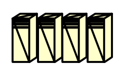
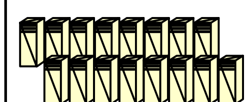
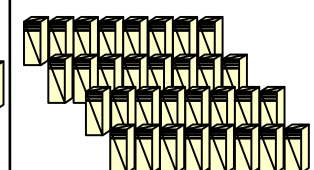
Operations (serial)



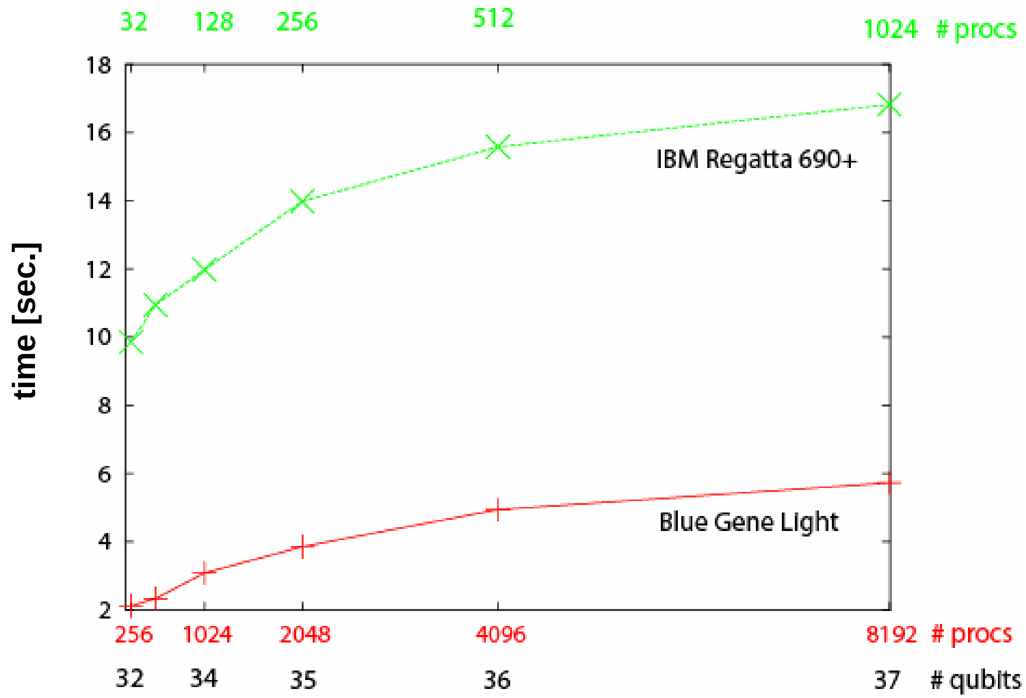
Operations (parallel)



Memory requirements

# qubits	32	33	34	35	36	37
# procs	32	64	128	256	512	1024
Memory statevector	64 GB	128 GB	256 GB	512 GB	1 TB	2 TB
Memory operations	96 GB	192 GB	384 GB	768 GB	1.5 TB	3 TB
# IBM p690 nodes						

Scaling Properties



- good scaling properties up to 37 qubits using 1024 (8192) procs and 3 TB memory
- highly efficient universal simulation code for gate level quantum computers

Operational Errors

Decompose operations into sequences of:

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \qquad P(\phi) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$$

$$H = R(\pi/4)\, P(\pi)$$

$$\text{NOT} = R(\pi/2)\, P(\pi)$$

introduce small deviations to the angles:

$$\theta' = \theta + \epsilon_\theta$$
$$\phi' = \phi + \epsilon_\phi$$

(Gaussian distributed with standard deviation σ)

Decoherence (a simple model)

Introduce with probability *p*/3 each

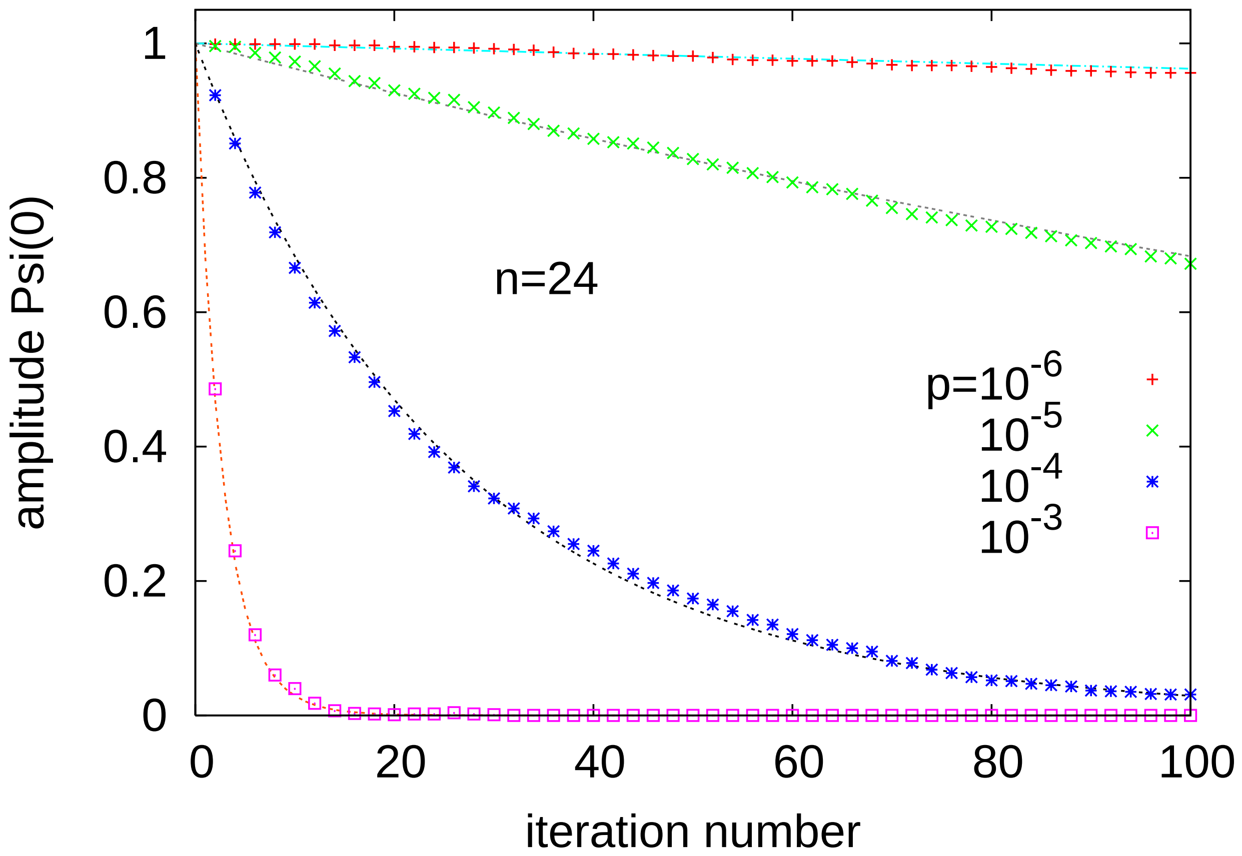
- bitflip $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
- phaseflip $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
- both $-i\sigma_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

with probability *1-p* $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

H^{2k}=1 Experiment

robustness of H^{2k}=1 to Decoherence

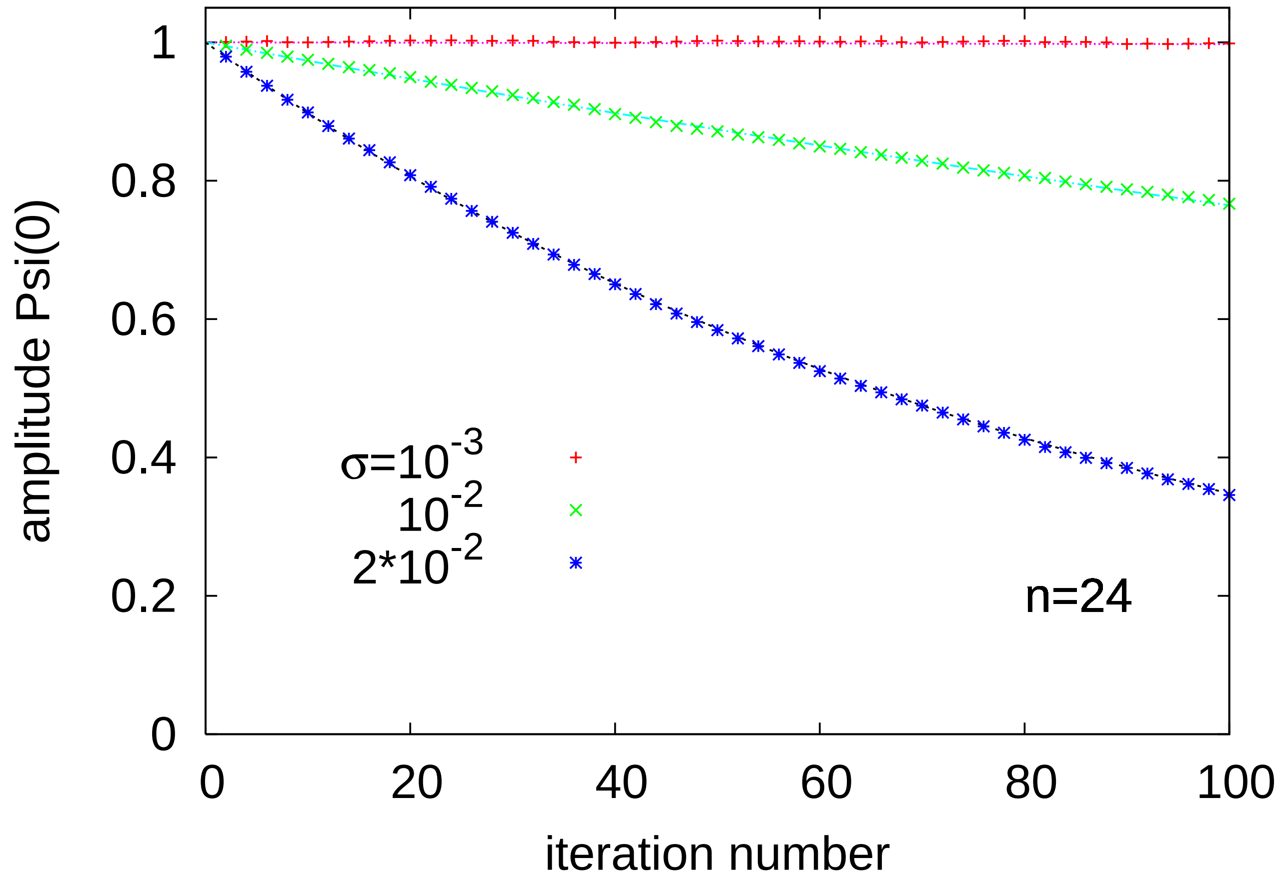
$$\psi_0 = |0\rangle\langle 0| = \left(\frac{1+(1-\frac{4}{3}p)^{nk/2}}{2}\right)^n$$



$H^{2k}=1$ Experiment

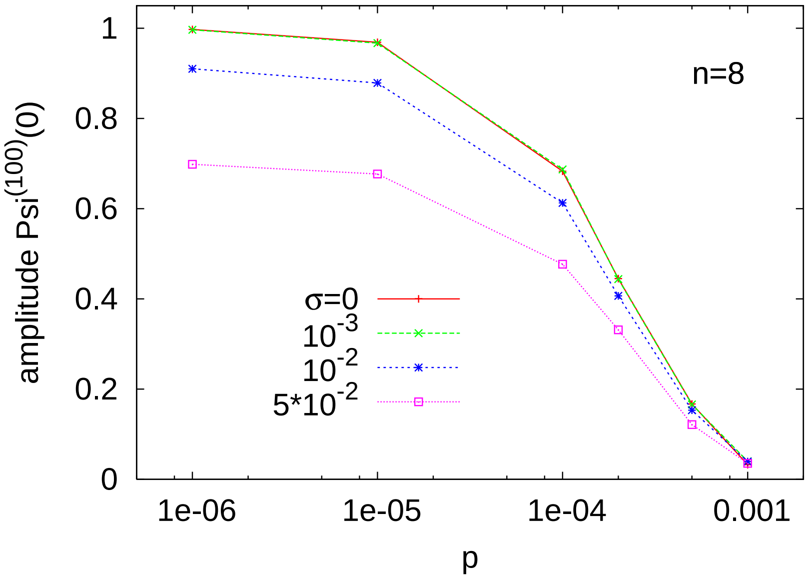
robustness of $H^{2k}=1$ to Operational Errors

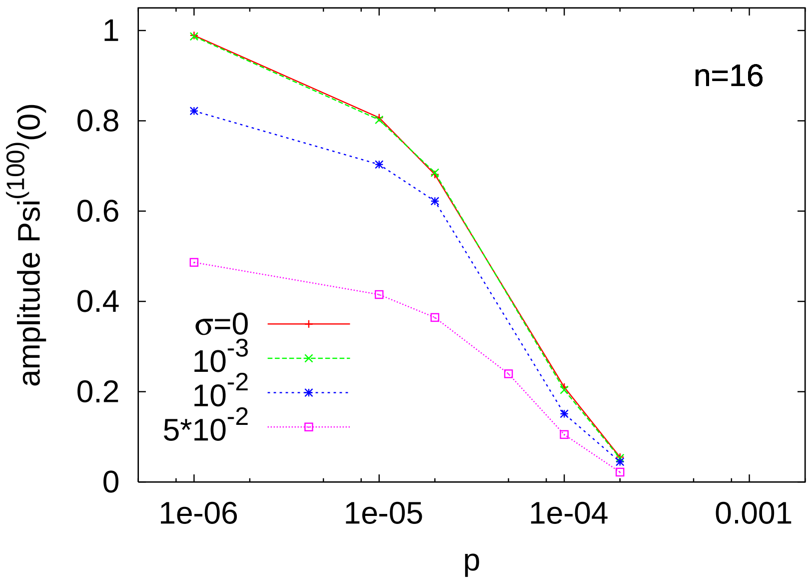
$$\psi_0 = |0\rangle\langle 0| = \left(\frac{1+e^{-\frac{\sigma^2}{2}9k}}{2}\right)^n$$

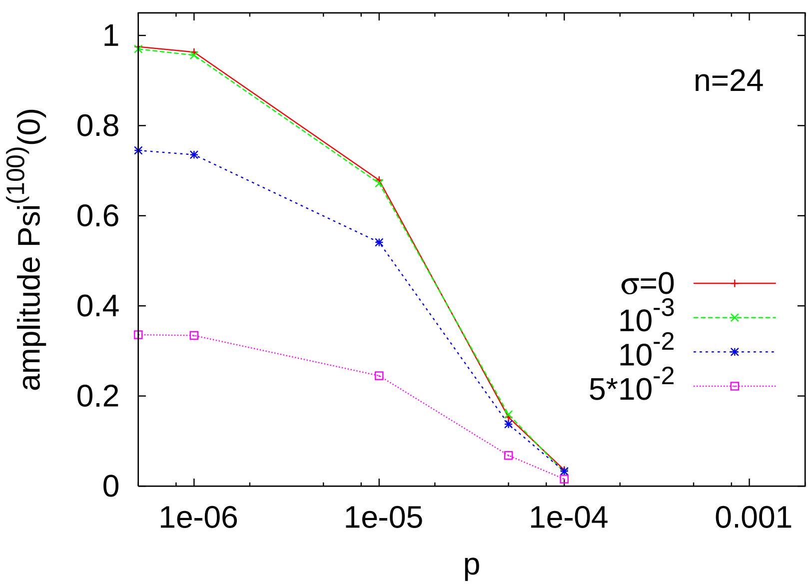


$H^{2k}=1$ Experiment

Dependence on system size

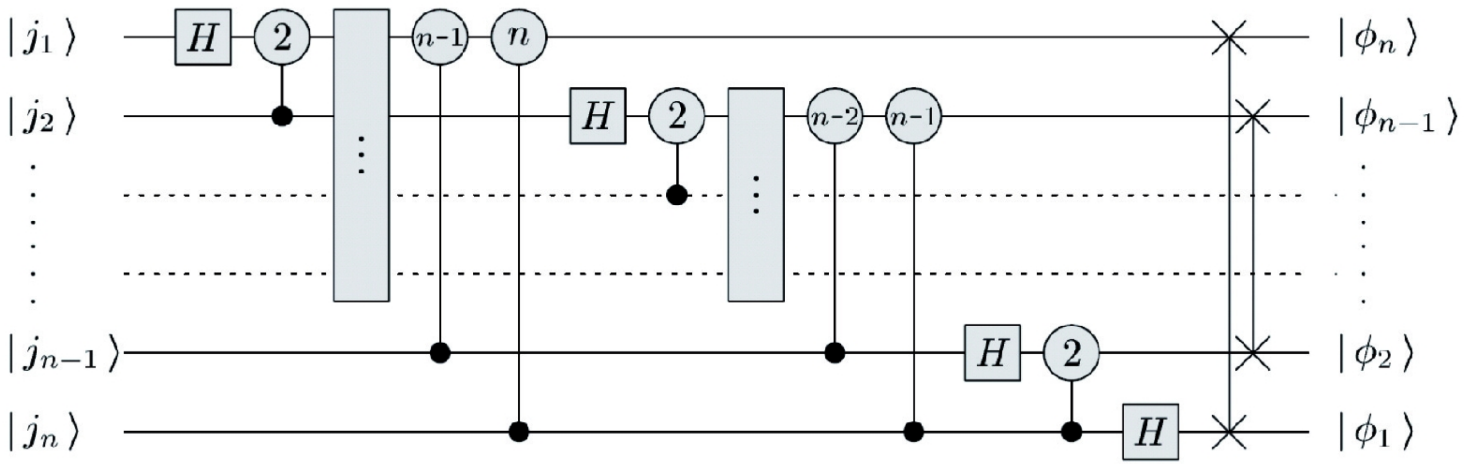






threshold $\sigma \approx 10^{-3}$

Quantum Fourier Transformation

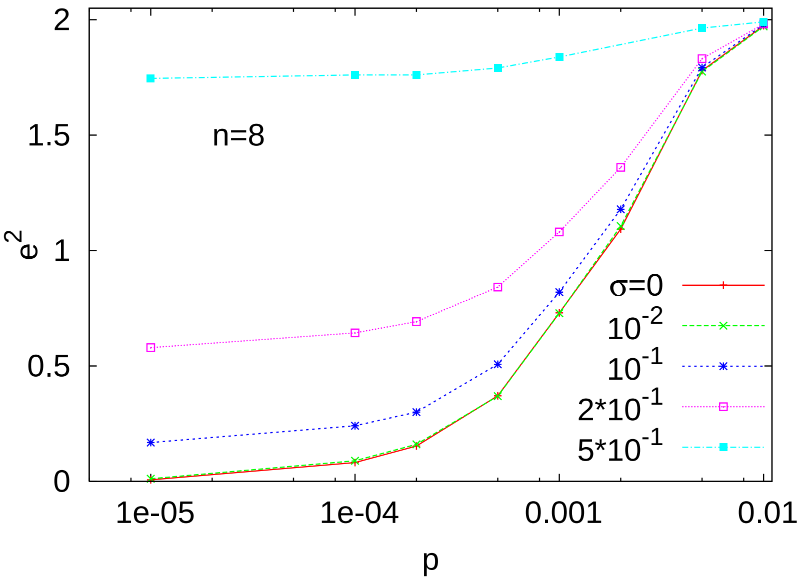


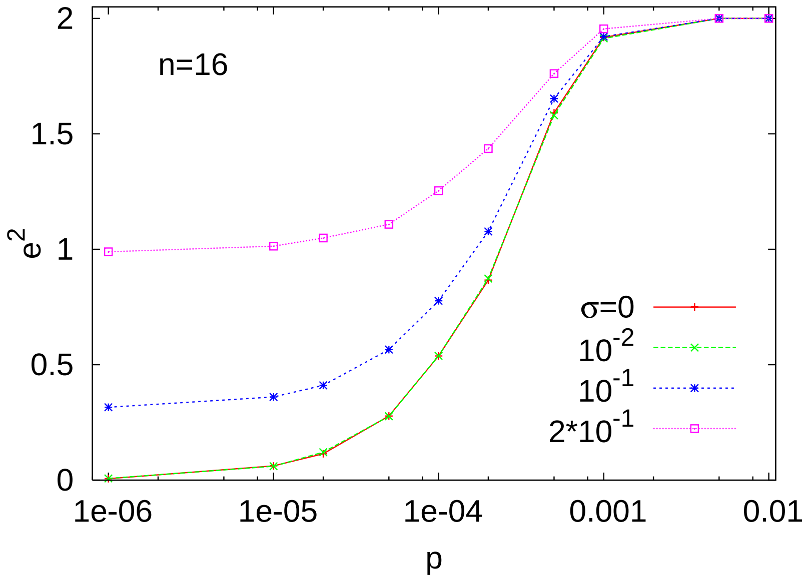
$$H_\epsilon^{(q)} = R_{\epsilon_1}(\pi/4)P_{\epsilon_2}(\pi)$$

$$SWAP(q_1 \leftrightarrow q_2) = CNOT(q_1,q_2)\,CNOT(q_2,q_1)\,CNOT(q_1,q_2)$$

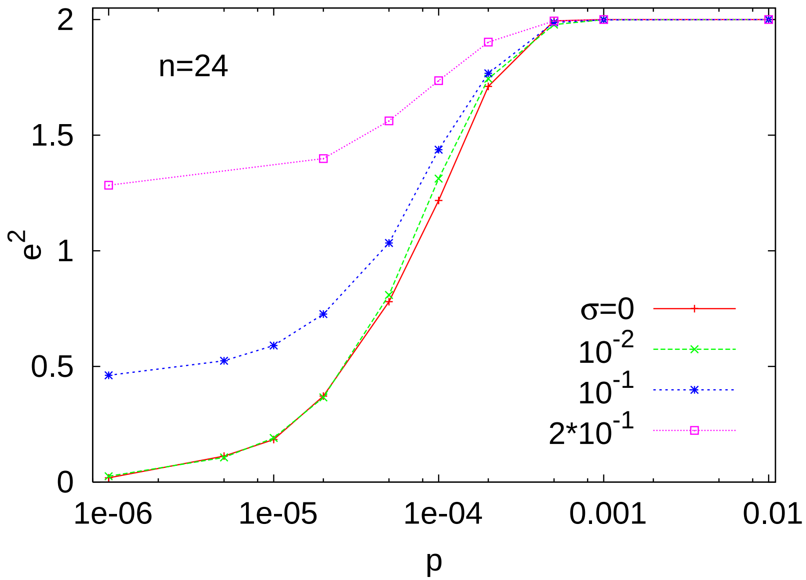
$$NOT_\epsilon = R_{\epsilon_1}(\pi/2)\,P_{\epsilon_2}(\pi)$$

Quantum Fourier Transformation





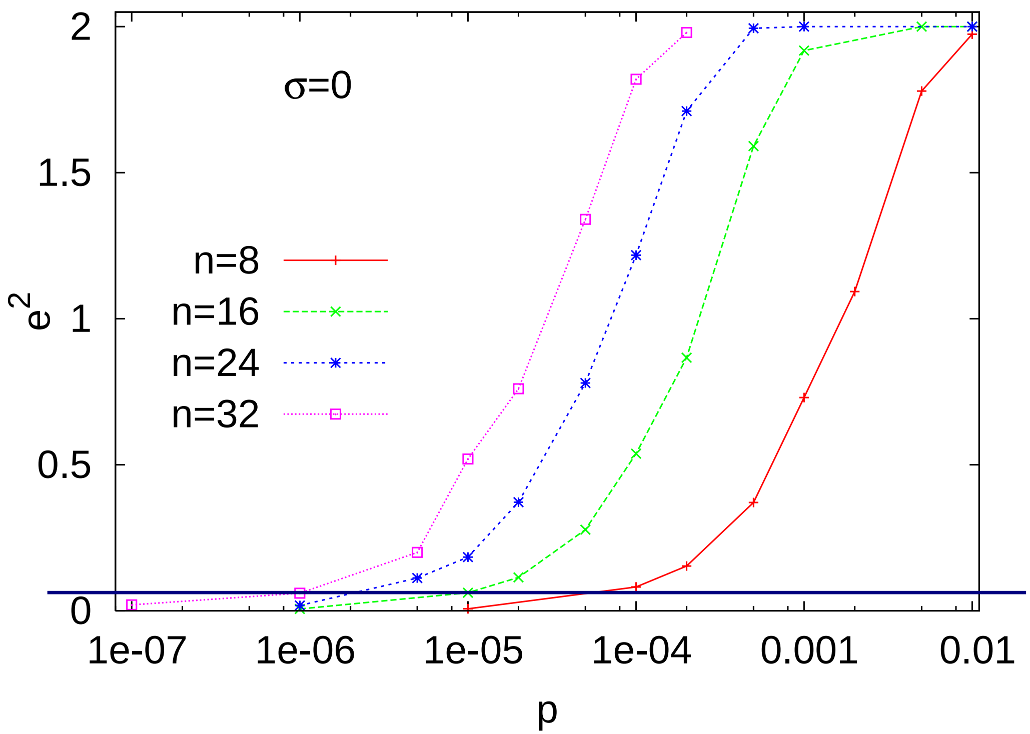
$$e^2(\sigma, p) = |\psi - \psi_{exact}|^2$$
with $0 \leq e^2 \leq 2$



threshold $\sigma \approx 10^{-2}$

Quantum Fourier Transformation

dependence of decoherence on system size:



system size n ⟶ 2n ⟹ p ⟶ 1/10 p

Quantum Fourier Transformation

Visualization of qubit "measurement"

- spin operator expectation values: $Q_\alpha = -\langle S_\alpha \rangle = -\langle \sigma_\alpha \rangle$

such that qubit state $|1\rangle$ is depicted by $\mathbf{Q} = (0, 0, +1)$

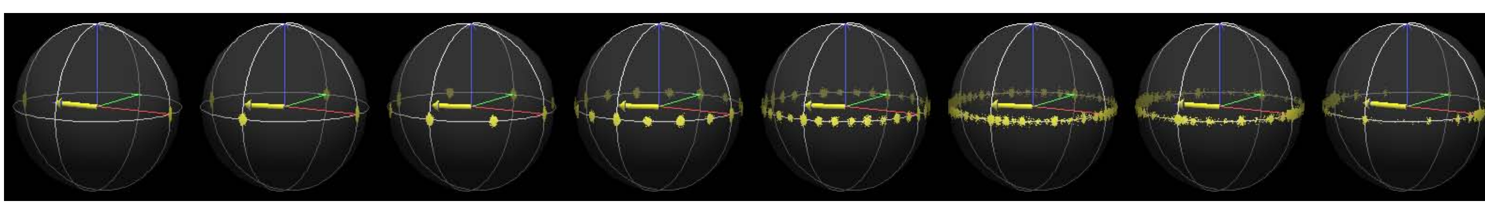
- ensemble average $\hat{\mathbf{Q}} = \sum_{i=1}^{m} \mathbf{Q}^{(\mathrm{i})}$

$$\mathbf{Q_8} = (-1, 0, 0) \xrightarrow{\sigma_\alpha} \mathbf{Q_8}' = -\mathbf{Q_8}, \mathbf{Q_8}$$

$$\mathbf{Q_7} = (0, 1, 0) \xrightarrow{\sigma_\alpha} \mathbf{Q_7}' = -\mathbf{Q_7}, \mathbf{Q_7}, -\mathbf{Q_8}, \mathbf{Q_8}$$

$p = 5 \times 10^{-3}$

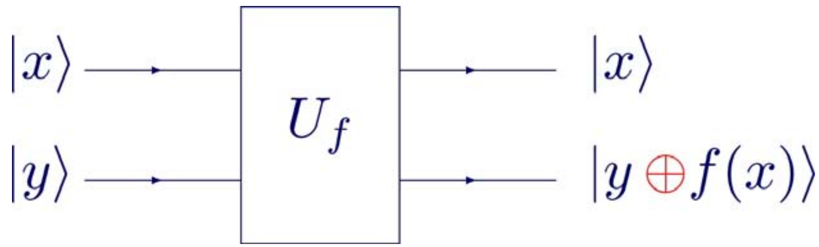
$\sigma = 10^{-2}$



Grover's Search Algorithm

Search an unstructured database of $N = 2^n$ entries

Oracle $f_k(x) = \delta_{kx}$



- **initialize**

$$|x\rangle \longleftarrow H\,|0\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} |j\rangle$$

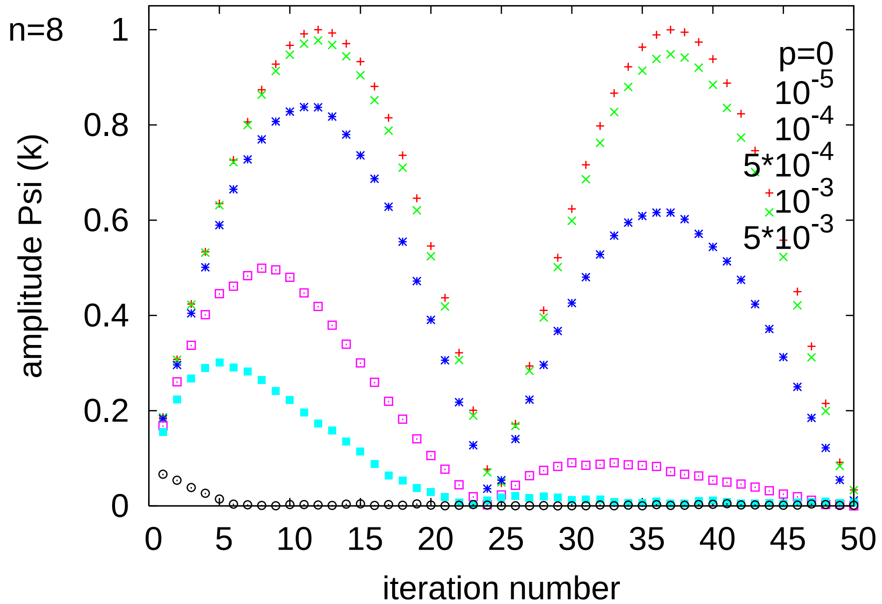
$$|y\rangle \longleftarrow H^{(0)} \sigma_x\,|0\rangle$$

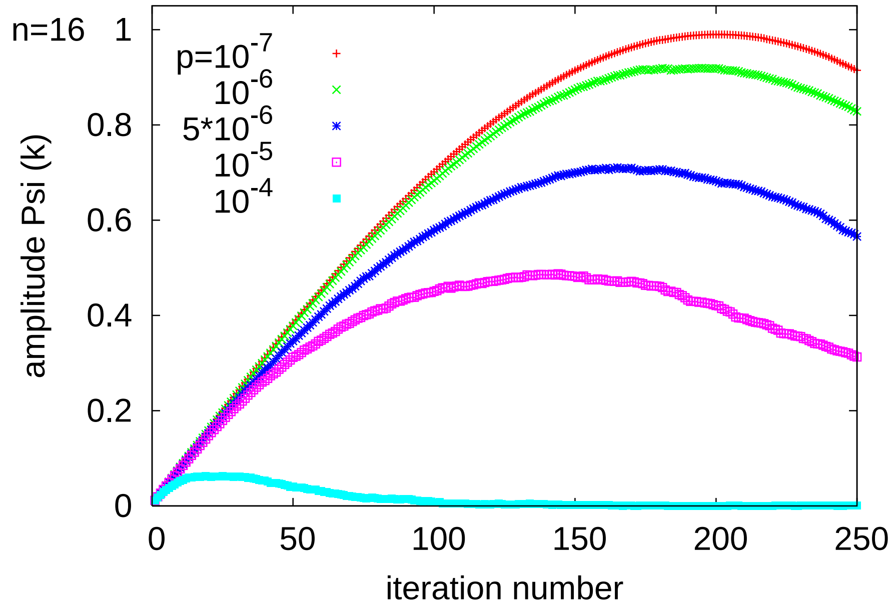
- **repeat until** $l \approx round\left(\frac{\pi}{4}\sqrt{N} - \frac{1}{2}\right)$

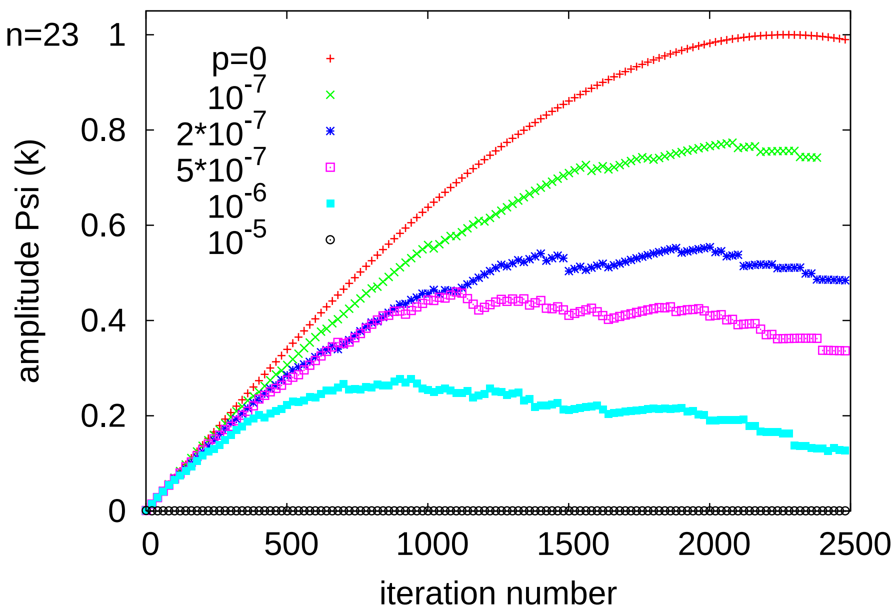
$$|\psi\rangle \longleftarrow Q|\psi\rangle = -HU_{f_0}HU_{f_k}|\psi\rangle$$

$$l \longleftarrow l + 1$$

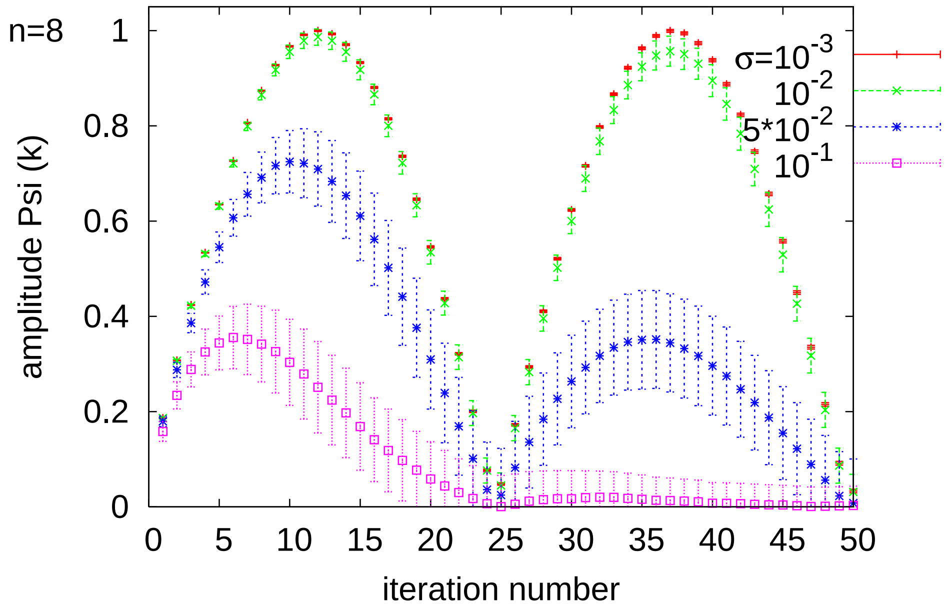
Grover (with decoherence)

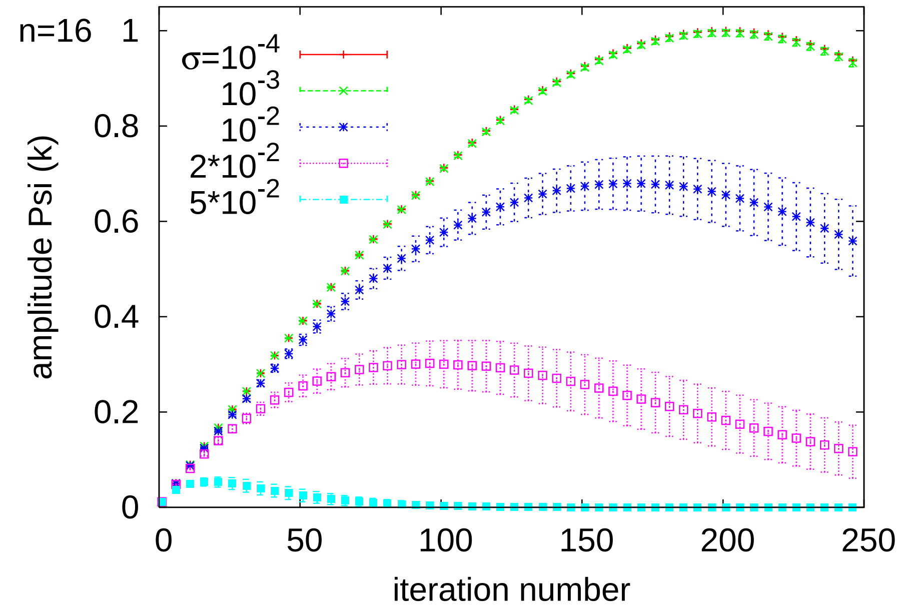


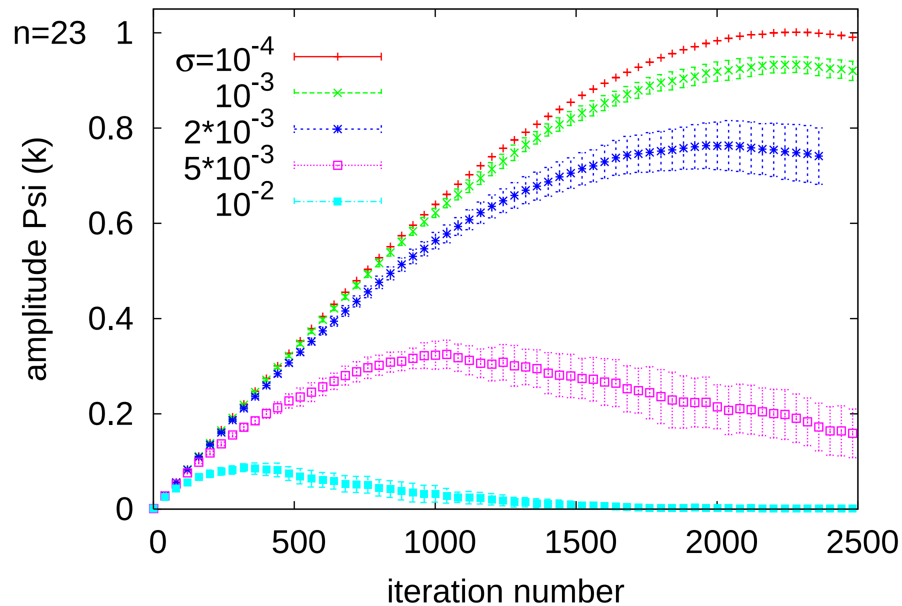




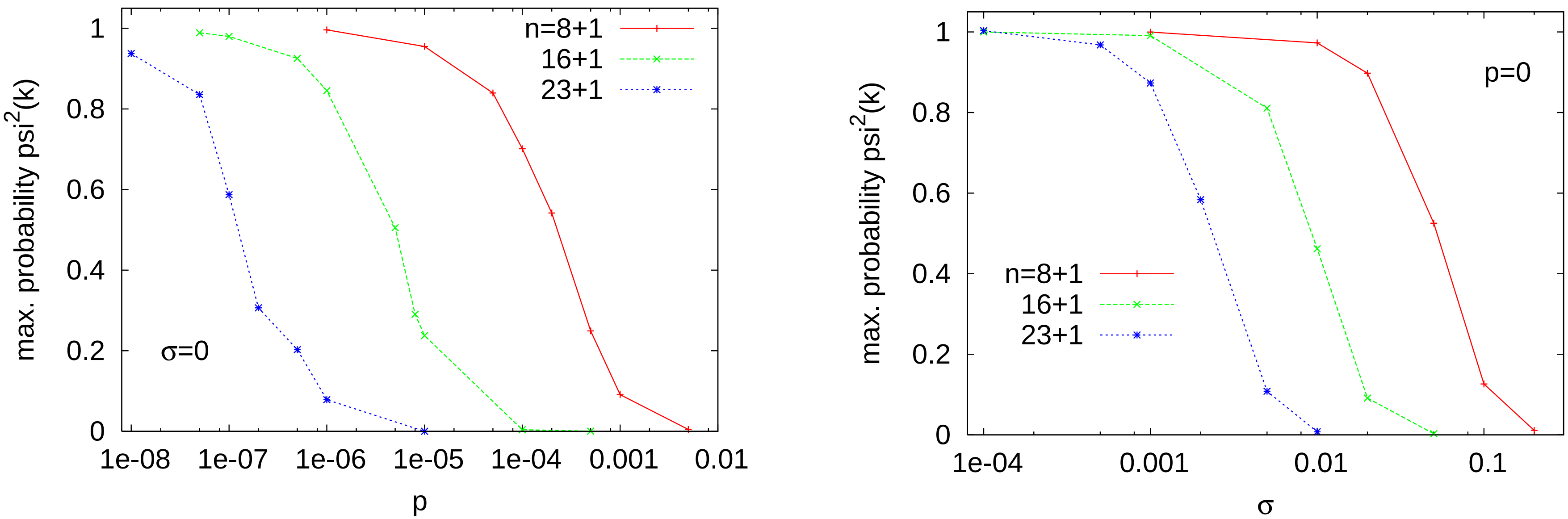
Grover (with gate errors)





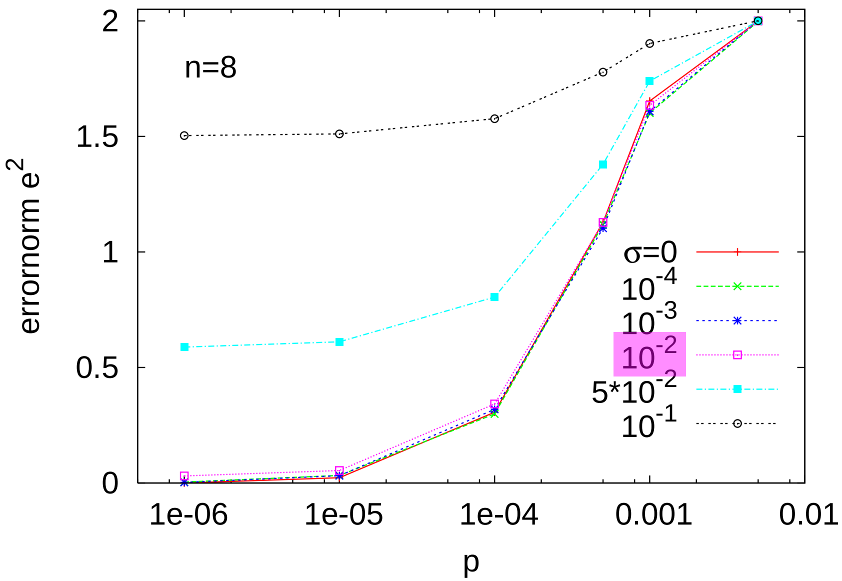


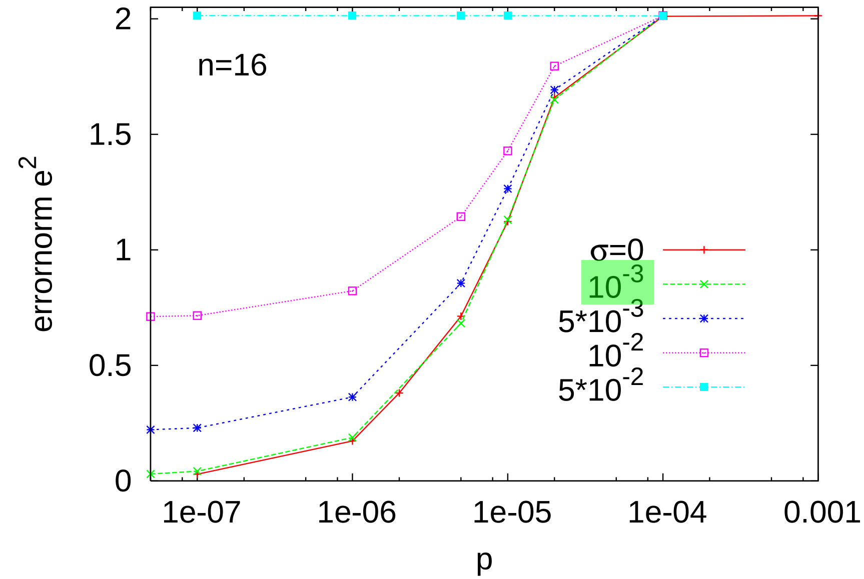
Grover (dependency on system size)



- error impact raises stronger with increasing system size than in case of QFT

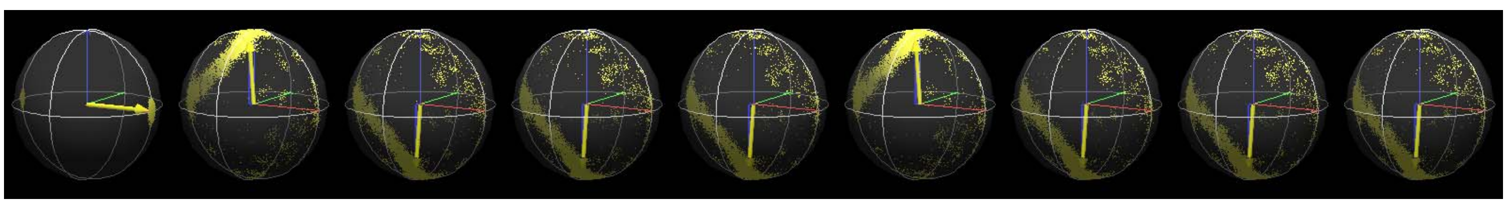
Grover (interplay of sources)





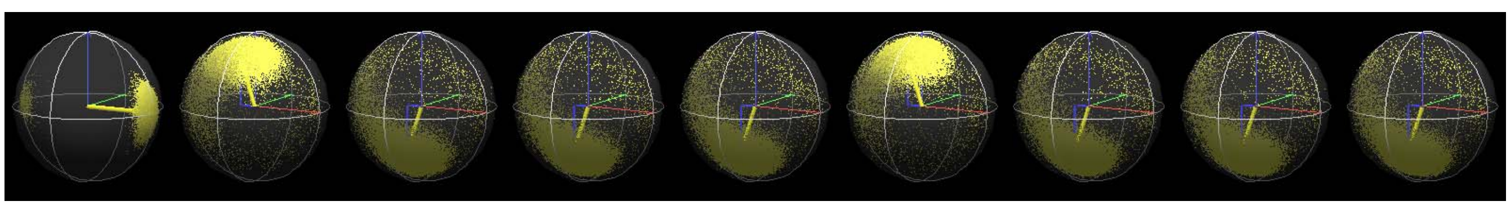
$p = 10^{-4}$

$\sigma = 10^{-2}$



$p = 10^{-4}$

$\sigma = 5 \times 10^{-2}$



Summery

- Basis: highly efficient + massively parallel QC simulator

- We have analyzed the impact of gate imperfections and decoherence errors within the idealized framework of QC simulation at gate level.

- We can quantify the dependency of the sensitivity to both error sources on the system size

- QFT more robust to operational and decoherence errors than Grover (and H^{2k}-Experiment)

- No hint on "destructive interference" of error sources

Outlook

- Scalability of Error Correction Schemes

- Realistic (=dynamic) simulations of ion trap quantum computer devices