Simulation of a Quantum Q-Byte system

EM Simulation

Team Members:

Harpreet Singh: Electro/Magnetostatics Solutions

Hunter Galeote: Time Independent SCE and Pauli's equation

Alexandre Proulx: Time Dependent SCE and Pauli's equation

Brendan Armstrong: Thermal simulation (Withdrawn).

Project Supervisor

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Overview and Background

"Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical" - **Physicist Richard Feynman**

In classical computers, a bit is a single piece of information that can exist in two states - 1 or 0. Whereas, Quantum computers uses 'qubits' which can exist in the superposition of states.

The Goal of our project was to simulate this alternate computing architecture that stores information as a function of the position of an electron. The project was divided into three parts: *Electromagnetism, Pauli's equation solutions,* and the *Time evolution*.

Motivation and Significance

- Currently, the processors are made on 22 nanometers process, and the transistor shrinkage is fast approaching a stop.
- With that, the end of Moore's law: *doubling of computational power every two years*.

" With Moore's Law running out of steam, quantum computing will be among the technologies that could usher in a new era of innovation across industries "- IBM

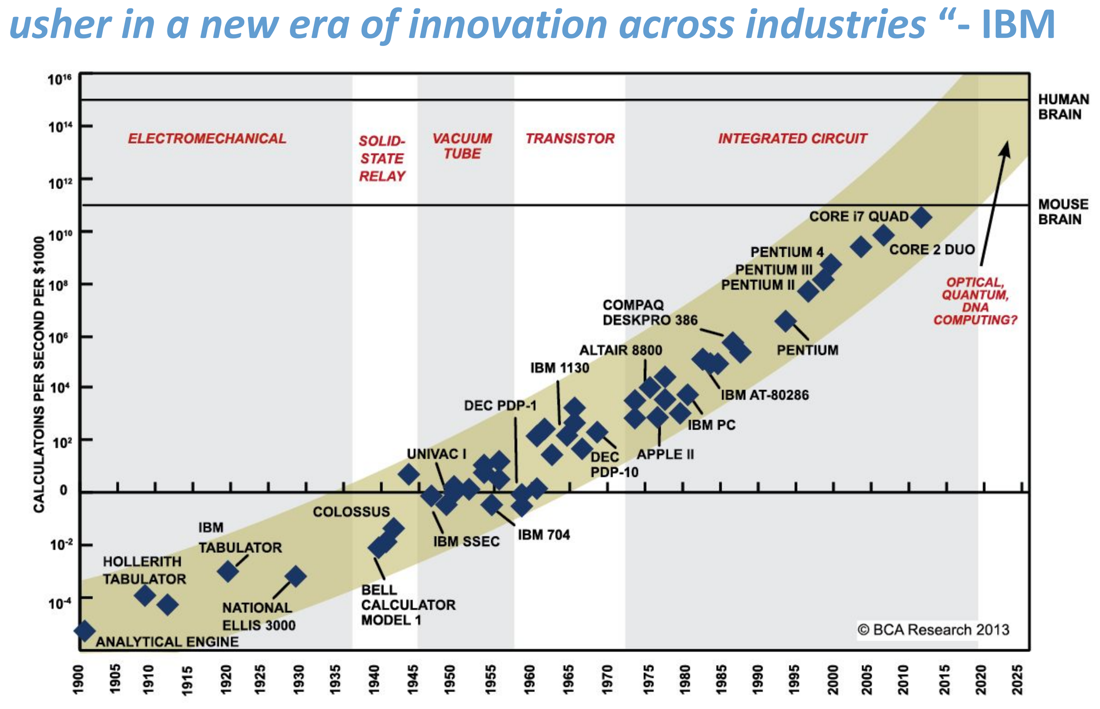


Figure 1: Moore's Law scaling.

- Faster than superfast computing, would make machine learning faster, along with the rapid progression of artificial intelligence.

Objectives and Specifications

- Our system consists of an electron and four wells,
- Magnetic field (B) is produced from a set of potential source configurations, such as current wires in X, Y and Z planes.
- The wave function was solved by feeding in Magnetic fields,
- Time evolution of our system is then performed to produce .gif
- Manipulating B field influences the position of an electron which is reflected in E field results.

General Approach and Theory

- Pauli's Equation (Spatial probability distribution):

$$\hat{H}|\psi> = \left(\frac{1}{2m}\left(\vec{\sigma}\cdot(\vec{p}-q\vec{A})\right)^2 + q\phi\right)|\psi> = i\hbar\frac{\partial}{\partial t}|\psi>$$

- Transient Equation (Time evolution):

$$\hat{\psi}^k = \left(1+\frac{i\Delta t}{\hbar 2m}\hat{G}\right)^{-1}\left(\hat{I}-\frac{i\Delta t}{\hbar 2m}\hat{G}\right)\hat{\psi}^{k-1}$$

- Ampere's Law (Magnetic potential sources):

$$\begin{bmatrix} \nabla^2 V_{Ax} = -uJ_x \\ \nabla^2 V_{Ay} = -uJ_y \\ \nabla^2 V_{Az} = -uJ_z \end{bmatrix}$$

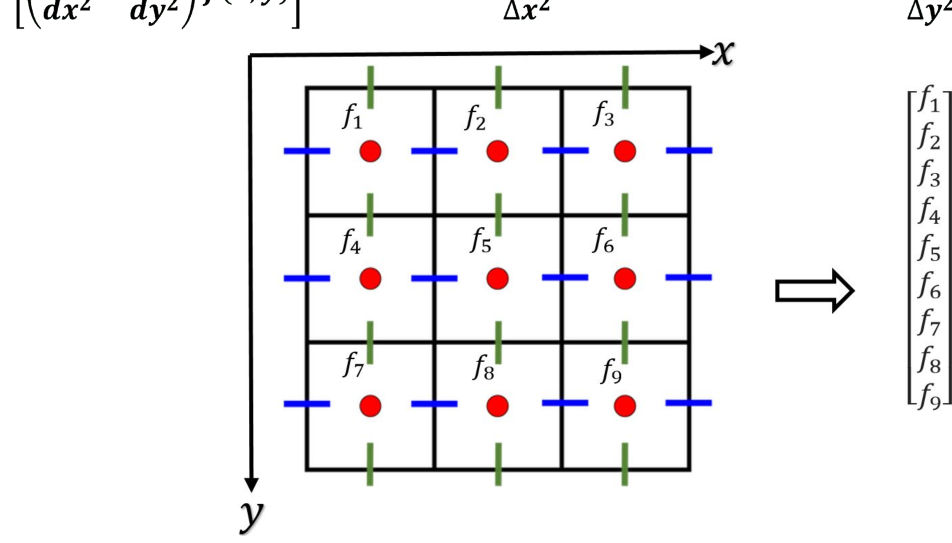
- Gauss's Law (Electric field distribution):

$$\nabla^2 V = \frac{-\rho_v}{\varepsilon}$$

Methods and Techniques

The finite-Difference method solves our continuous potential functions by discretizing it into a finite number of points over the region of our interest.

$$\left[\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}\right)f(x,y)\right] = \frac{f(j+1)-2f(j)+f(j-1)}{\Delta x^2} + \frac{f(k+1)-2f(k)+f(k-1)}{\Delta y^2}$$



Approximating second-order derivative using finite difference approach.

$$\frac{1}{\Delta_x^2}\begin{bmatrix} -2 & 1 & & & & & & & \\ 1 & -2 & 1 & & & & & & \\ & 1 & -2 & (0) & & & & & \\ & & (0) & -2 & 1 & & & & \\ & & & 1 & -2 & 1 & & & \\ & & & & 1 & -2 & (0) & & \\ & & & & & (0) & -2 & 1 & \\ & & & & & & 1 & -2 & 1 \\ & & & & & & & 1 & -2 \end{bmatrix}\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \\ f_8 \\ f_9 \end{bmatrix} = \begin{bmatrix} (f_2-2f_1+f_0)/\Delta_x^2 \\ (f_3-2f_2+f_1)/\Delta_x^2 \\ (f_0-2f_3+f_2)/\Delta_x^2 \\ (f_5-2f_4+f_0)/\Delta_x^2 \\ (f_6-2f_5+f_4)/\Delta_x^2 \\ (f_0-2f_6+f_5)/\Delta_x^2 \\ (f_8-2f_7+f_0)/\Delta_x^2 \\ (f_9-2f_8+f_7)/\Delta_x^2 \\ (f_0-2f_9+f_8)/\Delta_x^2 \end{bmatrix}$$

Similarly, differential operator for derivative with respect to y can also be written in matrix form.

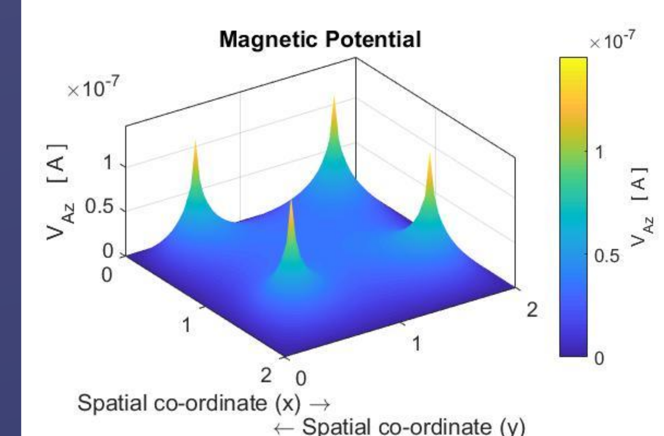
$$\frac{1}{\Delta_y^2}\begin{bmatrix} -2 & 0 & 0 & 1 & & & & & \\ 0 & -2 & 0 & 0 & 1 & & & & \\ 0 & 0 & -2 & 0 & 0 & 1 & & & \\ 1 & 0 & 0 & -2 & 0 & 0 & 1 & & \\ & 1 & 0 & 0 & -2 & 0 & 0 & 1 & \\ & & 1 & 0 & 0 & -2 & 0 & 0 & 1 \\ & & & 1 & 0 & 0 & -2 & 0 & 0 \\ & & & & 1 & 0 & 0 & -2 & 0 \\ & & & & & 1 & 0 & 0 & -2 \end{bmatrix}\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \\ f_8 \\ f_9 \end{bmatrix} = \begin{bmatrix} (f_4-2f_1+f_0)/\Delta_y^2 \\ (f_5-2f_2+f_0)/\Delta_y^2 \\ (f_6-2f_3+f_0)/\Delta_y^2 \\ (f_7-2f_4+f_1)/\Delta_y^2 \\ (f_8-2f_5+f_2)/\Delta_y^2 \\ (f_9-2f_6+f_3)/\Delta_y^2 \\ (f_0-2f_7+f_4)/\Delta_y^2 \\ (f_0-2f_8+f_5)/\Delta_y^2 \\ (f_0-2f_9+f_6)/\Delta_y^2 \end{bmatrix}$$

However, the right-side of our equations cannot be generalized and hence, we had to build matrices on a case by case basis.

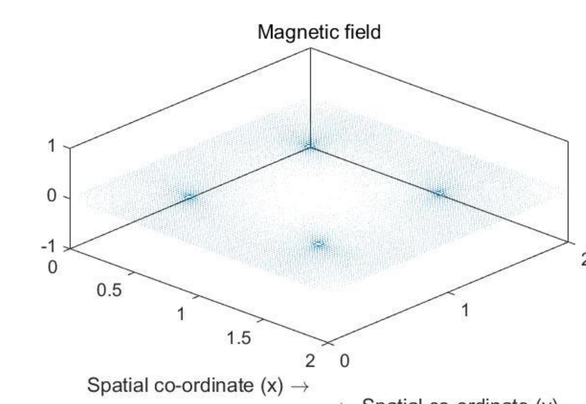
Challenges and Solution

- Incorporating material properties into our system was one of the challenging parts.
- The solution to the problem was changing the matrix approach to solve for differential equations to an iterative (or step by step) approach.
- The new approach did not discard the previous implementation but much of the part was built on it.

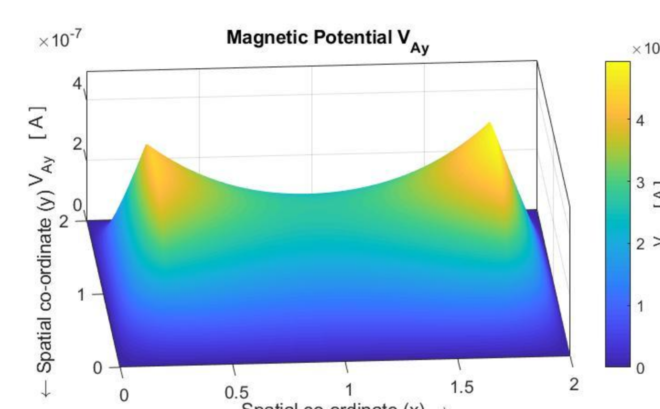
Results: Magnetostatics



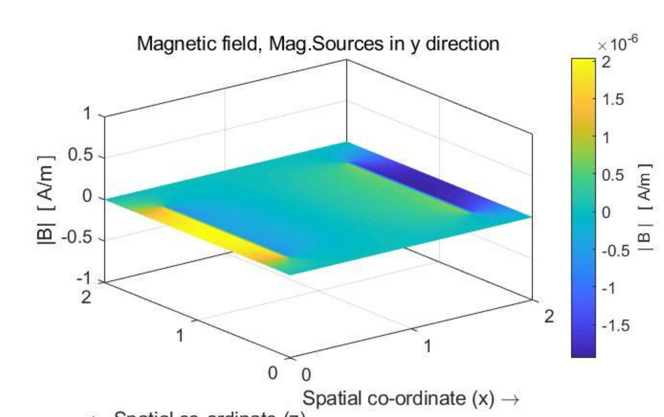
Magnetic Potential due to four current density poles.



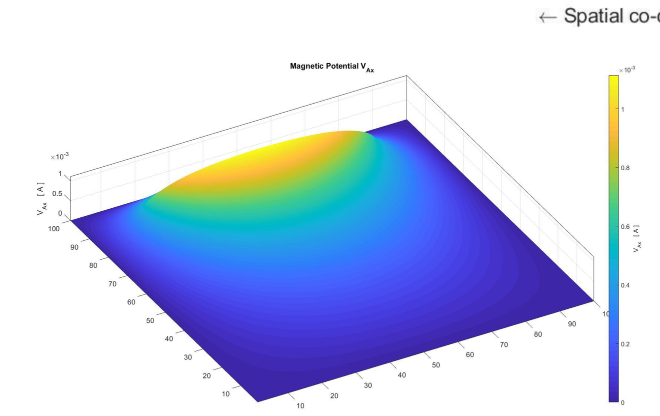
Magnetic-field due to four wires along z-direction.



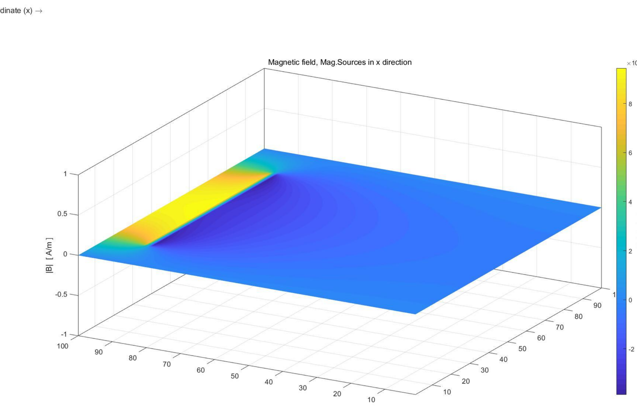
Magnetic Potential due to two wires in y-direction.



Magnetic-field due to wires along y-direction.

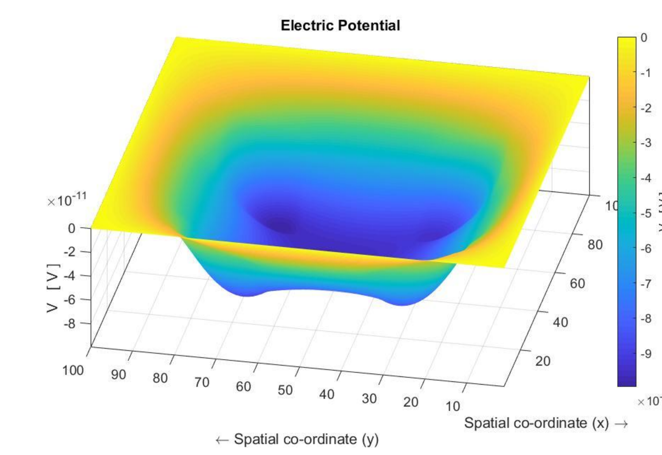


Magnetic Potential due to a wire in x-direction.

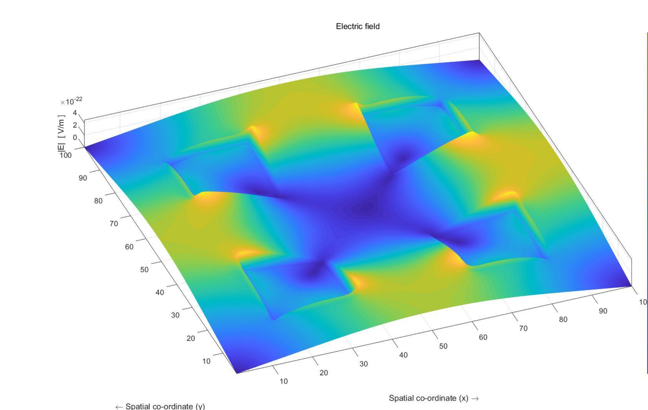


Magnetic-field due to a wire along x-direction.

Results: Electrostatics



Electric Potential with charge distribution as a square of wave function.



Electric fields due to the charge distribution.

Discussions

- The objective of our project was to build a 2D simulation for a system of one electron and four quantum wells,
- Plots shown here are a proof that the objective of our project has been accomplished in due time.
- The magnetic field produced by potential sources indeed influences electron's position.
- For our chosen material that is Silicon (Si) and Silicon dioxide (SiO2), we see that Material properties do play a significant role in the case of Electrostatics.

Future Work and Extension

- In a real-world scenario, thermal fluctuations are the key aspect that plays a crucial role when exploiting quantum properties of a system,
- Our simulation can be fabricated on a silicon wafer, and be tested to replicate the results obtained in simulation,
- Further research can be done on converting the existing system to a real-time system.

Contributions

- Hunter Galeote provided input data for electrostatics that is solved *Pauli's equations* to give wave functions for different Magnetic source configurations,
- Alexandre Proulx laid down architecture for geometry and performed *time evolution* of the system,
- Brendan Armstrong (Withdrawn) was to simulate thermal fluctuations.

References

- Figure [1]: *Graham Templeton*, "What is Moore's Law?", Extreme Tech, July 29, 2015.
- Prof. Tom Smy, *Electromagnetic Simulation*, The Physics and Modeling of Advanced Devices and Technologies.