



Department of Physics Research Experience for Undergraduates

Mathematica Vs. FEMLAB

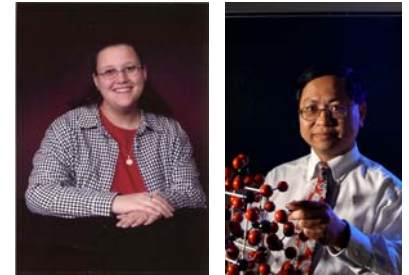
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Introduction:

The purpose of this project was to use two computer programs, Mathematica and FEMLAB, to solve a self-consistent Schrödinger-Poisson problem. The Poisson Equation is used to find the electric potential of given charge distributions. The Schrödinger Equation is used in quantum physics to predict the physical behavior of small nano-systems. In this case, the Schrödinger equation is used to solve a finite potential well problem; in the well there is an electron in a layer of GaAs.

Units: Length = nm
Mass = eV/c^2
Energy = eV

Both programs were run using a PC with: Pentium III processor, 3GHz, and 512 RAM.



Left: Paula Miller, Right: Dr. Lok C. Lew Yan Voon

Mathematica

Mathematica is a program used to solve complex mathematical problems. It has a wide range of uses from math to engineering to social sciences.

Pros:

- > It is a programming language, so it can be used for many different applications.
- > Has many different types of graphing capabilities.

Cons:

- Mistakes are easy to make and hard to find.
- Must have a great knowledge about the program to use it.

Procedure:

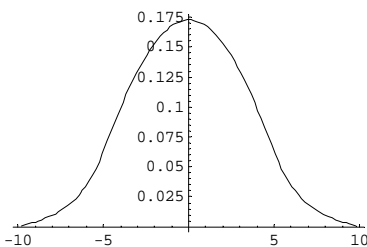
The procedures involved in programming this problem in Mathematica were very tedious. Solving an ordinary differential equation is difficult due to the fact that it is not a built in feature of the program. One must use the finite difference method to change the problem into a matrix and then solve for its eigenvalues.

Note: The following book was referenced for the procedure listed above. "Mathematical Methods Using Mathematica", by Sadri Hassani

Results:

The results obtained by mathematica were correct. However, the program took a long time to compute the solution and both the matrix dimension and the interval of calculation must be changed in order to obtain an accuracy to the third decimal place.

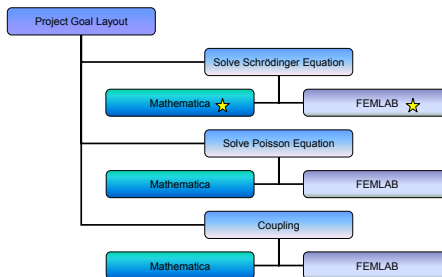
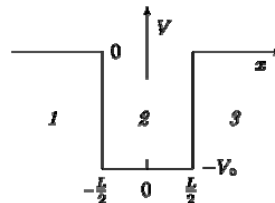
Ex.) When the interval of calculation was increased to around -200 to 200 and the numeric dimension of the matrix was increased to 2000, the numeric value went from .03229 to .03208. The program took approximately 19 seconds to perform this calculation. (the graph was too large to place in this poster so the graph for the interval of -10 to 10 was used.)



Conclusion:

Both Mathematica and FEMLAB are capable of performing complex calculations, however Mathematica is a little more difficult to use than FEMLAB. In FEMLAB, it is easier to obtain a good accuracy in the calculations than with Mathematica. FEMLAB also understands the physics of the problem so it is more applicable for this problem. One would have to conclude that for this type of physics problem, a program geared towards solving scientific problems is more suitable to use.

$$-(\hbar^2/2m^*)(d^2\psi/dx^2) + V(x)\psi = E\psi$$



Further Research:

The next step would be to solve the Poisson Equation and then couple the two together. For Mathematica this will be difficult because one would have to figure out how to write a program for this. FEMLAB will be a little easier for the reason that it has a multiphysics feature which allows the user to enter the values and the computer does the rest of the calculation.

Graphs:

The graphs show the first energy level given by both programs. As one can see the graphs do match pretty well, so both programs are capable of performing the calculations needed to solve this problem.

FEMLAB

FEMLAB is an interactive program which can model any type of PDE. It is mostly used by scientists and engineers.

Pros:

- > User friendly, step by step process.
- > Has many different graphing capabilities.

Cons:

- Must have a great knowledge of science and math to use efficiently.
- Only uses PDE forms of equations.

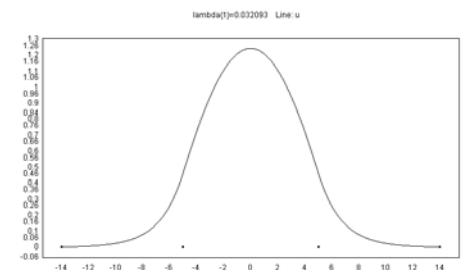
Procedure:

The procedures involved in programming the problem in FEMLAB were not too hard. The program already has the equation programmed into it. All the user must do is select the type of problem one needs to solve. The rest of the procedure took some research to find out how to enter in all of the numeric values.

Results:

The results obtained using FEMLAB were accurate. Not only was the numerical value correct, but the changes made in the interval of calculation produced an extremely accurate value to the third decimal place.

Ex) When the interval of calculation was increased the numeric value went from being .0322 to leveling off at .03209. The program took .035 seconds to perform this calculation.



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- ❖ Dr. Doug Petkie Assistant Professor (Department of Physics)
- ❖ Dr. Lok C. Lew Yan Voon Professor and Chair (Department of Physics)