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Learning Quantum Physics Building Simulations

Abstract Our experience on teaching Physics at the 1st course of the Physics career at Murcia University using computers to build simulations, particularly some examples about Quantum Mechanic, is presented. Our students develop a systematic series of physics models covering different topics dealt with in the General Physics course. At the same time, the basics of building models with a computer is introduced along with the necessary numerical techniques involved. In this communication we shall present the way we use computers to teach Physics at this introductory level and some examples done by students about quantum mechanics, a particle in a box, a particle in a finite potential well, time dependent function state.

1. Introduction

"Simulation is now an integral part of contemporary science and is having a profound effect on the way we do physics. The ability to compute is now part of the essential repertoire of research scientists" [1]. We claim that simulations may have also a profound effect on the way we teach physics and the way students learn physics, the ability to compute is now part of the essential repertoire of students to *do* physics. This is now feasible thanks to authoring tools like Easy Java Simulations [4], LabVIEW, or facilities to program like Physlets . In the first course of Physics Studies at the University of Murcia we teach a General Physics course and an Introduction to Computational Physics and Simulation. Problems that are proposed at the General Physics course can be treated more efficiently thanks to interactivity, graphical capabilities and animation due to time dependent problems that simulations offer.

Our goals coincide basically with those of Gould, Tobochnik and Christian in his book [1]
1. To provide a means for students to *do* physics.
2. To give students an opportunity to gain a deeper understanding of the physics they have learned in other courses *(General Physics in our case)*.
3. To encourage students to "discover" physics in a way similar to how physicist learn in the context of research.
4. To introduce numerical methods and new areas of physics that can be studied with these methods.
5. *(In our case we change this item)* To treat subjects that are complex to face them without computing techniques because their mathematical complexity.

After eight years teaching General Physics and an Introduction to Computational Physics and Simulation we can claim that the addition of both subjects is an efficient way to initiate pupils in the development of physics models. After some training, students are able to operate with a high variety of physical problems, and to handle situations with an analytical complexity higher than their mathematical background [2, 3]. By using computers, the learners can concentrate their effort in the model and numerical algorithms to solve the equations related to the problem.

To model and to create a simulation we use Easy Java Simulations (Ejs) [4], an authoring graphic tool developed for the conceptual learning of physics which allows the creation of

sophisticated interactive animated interfaces with not too much programming effort. Ejs is a Java application and produces Java applets that can be used alone or embedded in a web page that can also be built with Ejs, this tool implement the schem *MODEL-VIEW-CONTROLLER* [1] that separates the physics (model) from the user interface (the controller) and the data visualization (the view) that facilitate good design.

Simulations can be used to improve the teaching-learning process in quantum mechanics, an abstract and complex subject; *Physlets Quantum Physics* [5] uses over 200 ready-to-run interactive exercises which use over 250 carefully-designed computer simulation for the teaching of quantum physics. Our approach is different and complementary to the method shown. We propose to develop the simulations by the own students; this is feasible thanks to tools like Ejs that facilitate building sophisticated graphic interfaces with the use of the mouse. This tool demands little knowledge of programming; with one or two sessions of two hours our students become familiar with it. Based on our experience, we present here some general comments about our method and with more detail the part of our course corresponding to some basic quantum mechanics examples.

2. Subject development

Our students must develop three different and complementary aspects at the same time:

First, they will learn to model simple physics problems with an increasing complexity. The process has three main steps

- mathematically plan the problem
- identify the equation describing the process evolution
- compute numerically these equations

Student does not know any numerical method for solving differential equation; therefore it is necessary to teach one. During the first two or three lessons, the basic concepts of finite differences method are presented. At this point we pay special attention to the relation between the intervals of temporal discretization and the characteristic times that characterize the physical process.

The second aspect to develop is the use of programming tools, such us arrays, loops, logical sentences, subroutines and the use of mathematics libraries. It is important the presence and cooperation with a course devoted to introduce the basic concepts in computer science.

The last element to consider is the development of graphical interfaces that facilitates the understanding of a physical process. The students are initiated by the representation of motion in 2D. The graphical interface are growing in complexity by including plots, movable elements, arrays, springs, scalar and vector fields, etc. The creation of interactive interfaces allows to change the conditions of the model and to obtain data from the simulation that makes it possible to use the simulation as a virtual laboratory.

3. Materials

During the last years, we have learnt that the students, by themselves, tend to concentrate their attention and work into the development of attractive interfaces, missing the importance of the physics content of the model. The teacher should take care of this problem and prepare strategies to present a simulation as an opportunity to deep in the physics related knowledge. With this in mind, we have incorporated some educational elements. For instance, each student must have a notebook, analog to the one used in an experimental laboratory, where to take note about the physics of the problem, new programming elements and graphical design.

We have observed that computers enhance the participation of the students; they are interested to simultaneous search of information by Internet on the subject under study. In this field, we try to foster the critical analysis of the data obtained through internet in the immense world of the web where everyone writes about everything.

We have incorporated a questionnaire to be filled with the help of the simulation to be built. This new feature was very well accepted by the students and it has produced a double benefit: the students have concentrated their attention into the physical aspects of the simulation and it has established a greater connection with the FG course. The questionnaire makes also possible to stand out the most important physical aspects. The students of the first year do not reach enough maturity as to value the possibilities of the constructed model. At the end, the student have to make a report in the form of a HTML document including the basics of the phenomenon under study, information about the simulation itself, the answer to the questionnaire and the java applet simulation

In addition to the general development of the course, the pupils choose a subject to make a more advanced and detailed simulation, selected depending on their own initiative and personal capacity. The work is presented and defended in class, and is made available to the rest of the pupils. This is an important part of the program and a valid tool to foment the initiative of the student, to stimulate the curiosity by the physics and to develop the capacity of oral expression and critical analysis, since they can comment the work of other students.

4.   Particle in a box

We begin with the simplest problem, a particle in a box, in one dimension. We present here the problem of calculating the eigenvalues and eigenfunctions of the infinite potential well.

4.1 Theoretical introduction

Let us consider the motion of a single particle bouncing back and forth inside a box, from which it cannot escape, and without loses of energy when it collides with the walls of the box.

The time-independent Schrödinger equation in one dimension can be written as:

$$\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\varphi_E(x)+U(x)\varphi_E(x)=E\varphi_E(x), \forall x \qquad (1)$$

where we make use of an standard notation for Plank's constant, m is the mass of the particle, $\varphi_E(x)$ is the wavefunction and E the energy of the particle.

For the one-dimensional case, the function describing the potential well at each point can be written as:

$$U(x)=\begin{cases} 0, & \text{if } x\in(0,L) \\ \infty, & \text{if } x\notin(0,L) \end{cases} \qquad (2)$$

The equation (1) reduces to:

$$\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\varphi_E(x)=E\varphi_E(x) \quad \text{if } x\in(0,L) \qquad (3a)$$

$$\varphi_E(x)=0 \qquad\qquad\qquad \text{if } x\notin(0,L) \qquad (3b)$$

4.2 Numerical Resolution

We make use of the solution procedure reported in [6]. The box is divided into N+1 intervals Δx wide (Figure 1). The continuous eigenfunction $\varphi_E(x)$ will be evaluated in N+1 points, obtaining the array $\{f_i\}$.

Using finite differences, equation (1) writes as:

$$\frac{-\hbar^2}{2m}\frac{f_{i+1}+f_{i-1}-2f_i}{\Delta x^2} = Ef_i \tag{4}$$

So, the value of f at point i+1, f_{1+1}, is known in terms of the values at the two previous points:

$$f_{i+1} = -f_{i-1} + f_i\left(2 - \frac{2m}{\hbar^2}E\Delta x^2\right) \quad \forall i = 1, N \tag{5}$$

To solve the Schrödinger equation it is necessary to start with an initial value for E and to know f_0 and f_1. The wavefield must be zero in $x=0$ and $x=L$, eq (3b), i.e. $f_0=0$. We can assign any value for f_1. for instance $f_1=0.001$. The rest of the N-1 values are calculated by making use of (6). If a value $f_N =0$ is obtained, then E is an eigenvalue, and the array $\{f_i\}$ approaches to $\varphi_E(x)$.
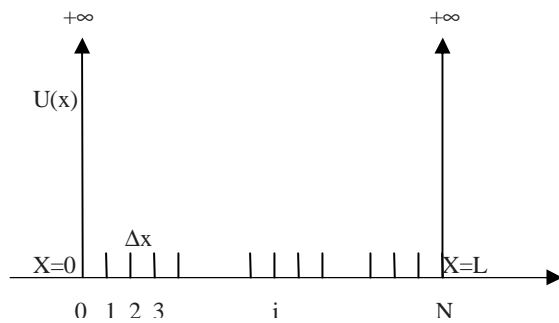

Figure 1. Spatial discretization of the infinite potential well

The method to calculate the eigenfunction φ_E and eigenvalues E, is the following [6]. We first begin with a small value of the energy and calculate the array $\{f_i\}$. Then the value of the energy is increased by ΔE and the new values for $\{f_i\}$ are recomputed. If we detect a change in the sing of f_N, then there must exist an eigenvalue of energy between E and E+ΔE. A better estimation of the exact value of the eigenvalue can be obtained by using a smaller ΔE.

Assuming $\hbar^2/2m = 1$, and $L = \pi$, the energy eigenvalues are described by:

$$E_n = n^2, \quad n = 1, 2, 3.... \tag{6}$$

4.3 Computer simulation

The student should develop a program using the Ejs programming tool to calculate the wave function depending on the energy. The simulation must include:
- A numeric field to introduce the energy

- An information field to present the value of f_N obtained by the computer.
- Two plots: f vs x and f^2 vs x.

As an example, Figure 2 is provided to the student. It shows a possible graphical interface. This simulation is developed at the middle of the course and the student has enough computational background to implement the numerical algorithm described above by themselves. As a help, we provide a possible list of variables Figure 3.
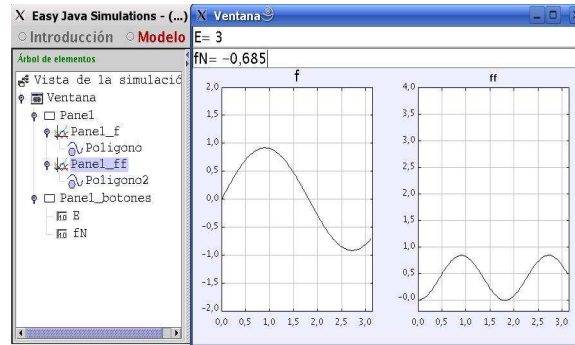

Figure 2. Graphical interface

Figure 3. Suggested list of variables

It is clear from the graphic representation that the functions that satisfy the boundary conditions are harmonic functions of the form:

$$\varphi_n(x) = A\sin(n\pi x / L) \tag{7}$$

for $0 < x < L$ with $n = 1,2,3..$

4.4 Questionnaire

Making use of your simulation, please answer the following questions:
a) Check the values $E=0.8$ and $E=1.2$, and plot the functions obtained
b) Found the first eigenvalue E_1. Plot the eigenfunction f_1 and the probability density f_1^2.
d) Plot the function for energy values slightly higher and lower than E_1. What do you find?, compare with case b)
c) Find the eigenvalues E_2 and E_3 and plot the corresponding eigenfunctions f_2 and f_3.
d) Coment the differences and similarities of $f_1 f_2$ and f_3

5. Particle in a potential barrier

In the above problem the analytical solution is not difficult and it can be reached by students which have worked previously with a similar differential equation when they study elastic forces, if we change the potential used in the previous section, modifying one of the

walls by a finite potential the analytical solution is not so easy as in the previous situation, here students can experiment the power of numerical calculation.

Now the boundary conditions changes at this wall, we must require the continuity of the function and the continuity of their derivative at this point.
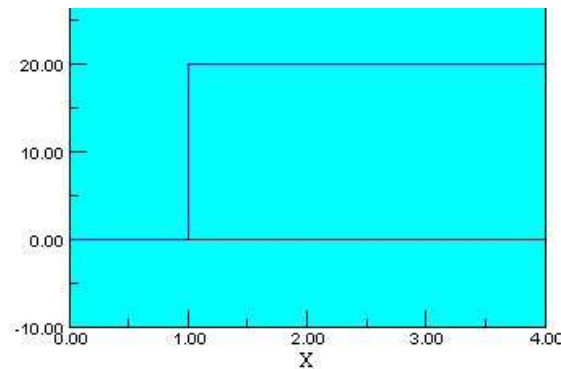

Figure 4. Diagram of potential energy, infinite energy at x = 0, and 20 at x = 1.0

We divide the x axis between energy walls in N equally spaced and we follow the calculus in other M points in the region of potential energy different from 0. The boundary conditions at the wall that separate the region with null potential energy with the region that has a non null value of potential energy, will be:
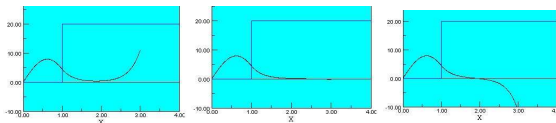
$$f[N+1] = 2 * f[N] - f[N-1]$$

Figure 5. Three steps of the search of a "possible" wave function modifying the energy that will result in a function that fits the boundary conditions.

Modifying the energy we test when it generates a function that fits all the boundary conditions. Figure 5 shows the step that allows to distinguish the eigenfunction.

6. Time dependent function state

The Schrödinger equation give us the time dependence of the wave equation, if we continue working with a problem in one dimension and with a potential energy function independent of time, we can write:

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) + U(x)\psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t} \qquad (8)$$

This function is complex, it will have a real part and an imaginary one, we can write:

$$\psi = \psi_r + i\psi_i \qquad (9)$$

If we substitute this equation in equation (8) we obtain a pair of equations, with the relate the real part and the imaginary part, both are very similar except in a sign.

Using finite differences similar to the development made at item *4.2 Numerical Resolution*, with a discretization of x shown at figure 1, and with the values, $\hbar/2m=1$, $L=\pi$, $dx=L/N$, we arrive at a pair of sentences that are ready for our computer:

In the case of $U(x)=0$;

$$fr[i]= fr[i]-(fi[i+1]+ fi[i-1]-2fi[i])dt/dx^2 \quad fi[i]= fi[i]+(fr[i+1]+ fr[i-1]-2fr[i])dt/dx^2$$

The general form of the solution of equation (7) can be expressed as a superposition of the eigenstates of the operator corresponding to any physical observable. If the Hamiltonian is time independent, we can write:

$$\psi(x,t) = \sum_n c_n \varphi_n(x) e^{-iE_n t/\hbar} \qquad\qquad (10)$$

If we are considering again the case of a particle in a box, we know that $\varphi_n(x)$ are eigenfuntions for the stationary states given by equation (7), we will use the following functions to begin the interaction:

$$fr[i]= c1\sin(n1\,x[i]\pi/L)+c2\sin(n2\,x[i]\pi/L)$$
$$fi[i]= 0$$

Where *c1* and *c2* are constants to be normalized and *n1* and *n2* are two quantum numbers. The student can observe that for $n_1 \neq n_2$ the quantum state changes through time with a time periodic constant; if *n1=n2,* the probability density function is stationary.
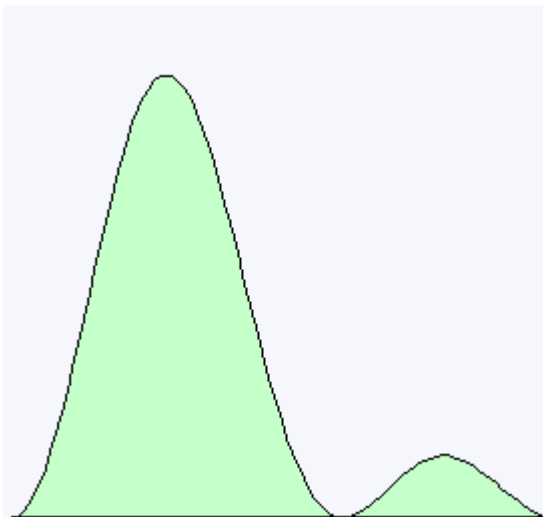

Figure 5. Density of states corresponding to a mix superposition in the infinite square well at a defined time.

7. Conclusions

The inclusion of an introductory course about Computational Physics and Simulation in the first year studies of Physics improve significantly the level of General Physics.

The use of simulations made by the own students motivate them, they becomes more active, they can face problems for what they are not yet mature because the mathematics they require.

Creating their own interactive simulation boost them to learn by searching.

Computer force students to think because it is very exigent, students must know very well the model to obtain the desired result.

8. Acknowledgements

9. References

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