

Lectures on Computer Assisted Modelling in Physics

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Abstract. *Our experience on teaching Physics at the 1st course of the Physics career at Murcia University, using computers to build simulations, is presented. This is carried out in a 60 hours practical Computer Laboratory course, in parallel with the General Physics course, both along a full 1st academic year in the Physics career. In the Computer Laboratory 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 program of this Computer Laboratory course together with some of the works done by our students*

Keywords. Computers in Physics Education; Physics Education Research, e-learning.

1. Introduction

The Spanish *withebook* for adopting the Bologna's indications in the field of Physics considers a physicist as professional of Science able to develop simple models in most of the fields [1].

One of the basic requirements of the Spanish *withebook* for the future Physics career is that numeric calculation that must be introduced in the obligatory course of Computational Physics. It will be also established an obligatory course of General Physics, devoted to introduce the most basic and general aspect of physics.

Both courses were already included in the present Degree of Physics at the University of Murcia. Six credits (60 hours) are assigned to Computer Laboratory (CL, Laboratorio de Física Computacional) and 15 credits (150 hours) to General Physics (GPh, Física General). All the students on Physics must attend to both courses along the full first academic year. In addition to

CL, there is another course related with numerical computation called Computer Science (Informática), where the student learn the basic aspects and systematic of programming science. CL was designed in order to enhance other transversal competences such as collaborative work, personal initiative, searching of literature and to develop speaking and writing communication.

After seven years teaching CL and GPh 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 modelling, numerical algorithms solve the equations related to the problem.

To model we use Easy Java Simulations (Ejs) [4], a graphic tool developed for the conceptual learning of physics which allows the creation of sophisticated interactive animated interfaces with not too much effort. Ejs is a Java application and produces Java applets that can be used alone or embeded in a web page that can also be built with Ejs.

Based on our LFC and FG experience, we present here the LECTURES ON COMPUTER ASSISTED MODELLING OF PHYSICS, as a course of a standard Physic Degree. It is initially designed to be taught in parallel with the General Physics course, during a full academic year. It can be easily adapted to one semester course for students with enough physical background.

2. Subject development

During the course, the 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
- numerically compute these equations

At that moment, students do not know any numerical method for solving differential equation; it is necessary, therefore, to teach one. During the first two or three lessons, the basic concepts of finite differences method are presented. In 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 as 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. Practices

During the course we develop, with this practical approach, a great part of the subjects treated in lectures. A list of the practices that can be made in a year is shown in Table 1. We can observe that all the subjects of an annual course of GPh are covered, in particular we deal with all the requirements for the future lecture on "Foundations of Physics": Newtonian, relativistic, quantum and statistic mechanics, electromagnetism and waves. During the academic year, the students are making their own database of simulations, which would be very useful to study, clarify aspects and test fundamental laws.

- 1- Apparent retrograde movement of planets.
 - Planetary model of Ptolomeo
- 2- Motion equations in 1D.
 - Forced and damped oscillation
- 3- Motion equations in 2D
 - Parabolic throw
 - Central acceleration
- 4- Relative motion. Reference systems. Centrifugal and Coriolis accelerations
 - The merry-go-round case
 - Equatorial long distance launching
- 5- Relativistic cinematic.
 - Muon decay
 - Twin paradox
 - Photon launching: Doppler effect
- 6- Dynamic of particles' systems
 - Gravitational interaction between 2 particles
 - The case of Sun-Earth-Moon
 - The limit of Roche
 - Gravitational chaos of 3 particles
 - Elastic interaction between 2 particles
 - Dynamic of the center of mass and internal particles??
- 7- Conservation laws (3D representation)
 - Gravity and conservation of angular momentum and energy.
 - Elastic forces and conservation of angular momentum and energy.
- 8- Relativistic mechanics
 - Momentum, force, energy and acceleration
 - Precession of perihelion
- 9- Statistical mechanics
 - Kinetic model of a gas
 - Pressure and temperature
 - Energy and velocity distributions
 - Brownian motion
- 10- Quantum mechanics
 - Energy in a potential box
 - Temporal evolution of the quantum state
- 11- Electromagnetism
 - Electric field of charges in a regular polygon
 - Motion of charges in magnetic field
 - Charges trapped in the terrestrial magnetosphere
 - Interaction between magnets
- 12- Waves
 - Propagation of blood-pressure pulse
 - Propagation of electromagnetic waves

Table 1. List of simulation

4. Materials

In order to obtain the maximum academic benefit it is necessary to establish a close correlation between CL and GPh courses. Therefore we always try to adapt the development of the CL course to the theory classes. By the CL and GPh coupling, the attention of the student is stimulated and the knowledge explained in Physics lectures is strengthened. The list of simulations is not closed. Many times it is useful to change a simulation or to include new ones. The temporal separation between theory and simulation is very important; we always try that it does not exceed of one week

The students have available some documentation for each specific simulation that includes:

- the presentation of the problem with the necessary numerical approximations
- a short description of the new features in programming, if any
- the contents for the graphical interface

The documentation of each simulation concerning to elements of programming, including some code, is adjusted to the students' abilities. Therefore, with the course the total amount of documentation is decreasing till the end of the year, when the students are able to model some problems without information about programming.

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.

This year 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 GPh 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.

5. Example: "Particle in a box"

For instance, we present here the problem of calculating the eigenvalues and eigenfunction of the infinite potential well.

5.1 Theoretical introduction

Let consider the motion of a single particle bouncing around inside an immovable 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 can be written as:

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

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:

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

The equation (1) reduces to:

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

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

5.2 Numerical Resolution

We make use of the solution procedure reported in [5]. 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:

$$\frac{-\hbar^2}{2m} \frac{f_{i+1} + f_{i-1} - 2f_i}{\Delta x^2} = E f_i \quad (4)$$

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

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

To solve the Schrödinger equation it is necessary to start with an initial value for E and to know f_0 and f_j . 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_i . for instance $f_i=0.001$. 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 $\varphi_E(x)$.

The method to calculate the eigenfunction φ_E and eigenvalues E, is the following [5]. 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

sign of f_N , then there must exist an eigenvalue of energy between E and $E+\Delta E$. A better estimation of the exact value of the eigenvalue can be obtained by using a smaller ΔE .

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

$$E_n = n^2, \quad n = 1, 2, 3, \dots \quad (6)$$

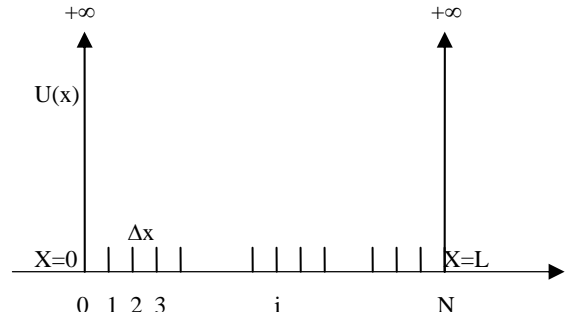


Figure 1. Spatial discretization of the infinite potential well

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

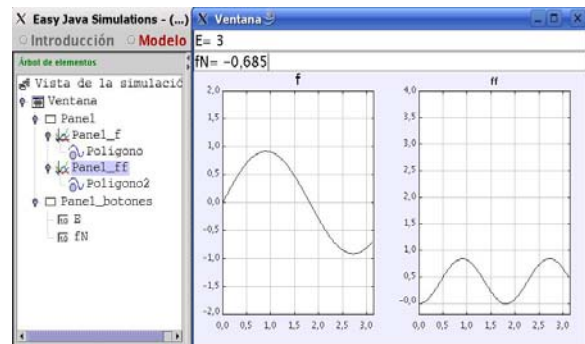


Figure 2. Graphical interface

Nombre	Valor	Tipo	Dimensión
L	Math.PI	double	
N	100	int	
dx	L/((double)N)	double	
x		double	N+1
f		double	N+1
E	0.8	double	
ff		double	N+1
fN		double	
m2_h2	1.	double	
		double	

Figure 2. Suggested list of variables

5.4 Questionnaire

Making use of your simulation, please answer the following questions:

- Check the values $E=0.8$ and $E=1.2$, and plot the functions obtained
- Found the first eigenvalue E_1 . Plot the eigenfunction f_1 and the probability density f_1^2 .
- Plot the function for energy values slightly higher and lower than E_1 . What do you find?, compare with case b)
- Find the eigenvalues E_2 and E_3 and plot the corresponding eigenfunctions f_2 and f_3 .
- Comment the differences and similarities of f_1 , f_2 and f_3

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7. References

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