



# STOCKHOLM UNIVERSITY

DEPARTMENT OF PHYSICS

IMPLEMENTATION OF COMPUTER AIDED  
LEARNING IN UNDERGRADUATE PHYSICS  
TEACHING

Flexible Learning in Physics

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## **Implementation of Computer Aided Learning in Undergraduate Physics Teaching**

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### **Abstract**

To increase the flexibility and efficiency of physics undergraduate teaching we have implemented the use of computer programs in the teaching of several physics courses. We have focused our interest on computer demonstrations covering a wide range of physics items, particularly modern physics like wave and quantum mechanics. The experience gained was used in the implementation of a new quantum mechanics course for chemistry students, where the use of the computer was implemented from the beginning. In addition special project works have been explored as a complement to the traditional examination forms.

### **1 Introduction**

The introduction of new teaching methods, such as a more systematic use of computers, involves changes in the way physics has been taught and in the teaching tools used. In particular new possibilities open up to demonstrate and illustrate difficult concepts and to aid the students to develop an intuitive picture of the material. The experience of the implementation of Computer Aided Learning in undergraduate physics teaching presented here is part of the Flexible Learning in Physics, FLIP project [1]. The aim is to increase the flexibility and efficiency of physics teaching and to introduce international character and co-operation into the educational program. This is an important part of making Swedish students internationally competitive and of making our teaching more attractive also to foreign students. We intend to achieve this by introducing the computer in the teaching and learning process in several physics courses. We have focused our interest on computer programs produced by the Consortium for Upper Level Physics Software (CUPS) [2], which has developed a comprehensive series of nine books and software packages. CUPS is an international group of 27 physicists, all with extensive background in the research, teaching and development of instructional software, that have been developing this series over several years. Each package is comprised of a paperback text and one or more diskettes. All of the computer simulations are provided in executable form. The individual chapters and computer programs cover mainstream topics that are found in standard textbooks for each course.

At the Department of Physics we have experience of using the CUPS programs in several courses, especially in mechanics, waves and optics and

quantum mechanics. During lectures the programs are run on a computer connected to an overhead projector and displayed on the wall, preferably with a high luminosity projector. The flexibility of the programs and the graphical capabilities coupled with the "advanced overhead projector" can give very instructive illustrations to the lectures which would be impossible with ordinary handmade overhead pictures or traditional black board drawings.

The work is concentrated on the following areas:

- the incorporation of interactive computer programs in some of the existing courses
- the introduction of special project work using the computer
- the exploration of alternative forms for student examination

## **2. Computer Aided Learning in the Mechanics and Waves and Optics Courses**

During the last 15 years the computer has gradually become a natural tool for the undergraduate students in science. Today a majority of the students at the Department of Physics have their own computer at home and all students have access to one at the department. When the computer was introduced into the undergraduate physics courses during the early 1970's first BASIC and later PASCAL was used in solving more advanced but not too difficult problems.

Today interactive program packages like MATLAB™ [3] and others which contain powerful numerical and graphical routines open up the possibility to treat problems more easily than before. Experience in handling MATLAB can be carried over to other program packages and is an important part of the undergraduate studies.

When students start their physics studies their background experience in handling a computer can vary very much. During the first year the students follow an introductory course in using WORD and MATLAB. This first course should thus guarantee a common minimum level for all students.

### **2.1 Use of MATLAB**

In the laboratory work MATLAB is constantly used for statistical treatment including least-squares fitting of theoretical expressions to experimental data and for error analysis. Graphical representations and diagrams are made with MATLAB and included into the final report which is written in WORD™. In some laboratory sessions the computer is used directly to collect and process experimental data. One example of such an experiment is a study of two coupled equal pendulums where the influence of the strength of the coupling on the behaviour of the two pendulums is studied.

Typical text book problems are usually limited to those which have an analytical and not too complicated solution. The powerful numerical routines of MATLAB make it possible to solve more complicated and realistic problems that cannot be treated in traditional problem solving sessions. In several courses the students are given problems on more

advanced level which need numerical methods to be solved. Typical such problems may require numerical solution of ordinary differential equations and systems of differential equations, evaluation of non-elementary integrals and computation of eigenvalues and eigenvectors of symmetric matrices. In the course Waves and Optics the Fourier Transform (FFT) routine in MATLAB is used.

## **2.2 CUPS Programs in Mechanics and Waves and Optics Courses**

Many of the CUPS programs illustrate phenomena in animated form which are very instructive in for instance mechanics and wave motion. In most programs the effect of varying important parameters can be studied. The programs can also be used to find numerical solutions to more difficult problems, for instance to find the frequencies of the normal modes of a complicated system of coupled oscillators. So far the CUPS programs have been used mainly by the teachers to give advanced illustrated examples in lectures, but the CUPS programs are also available to the students for individual training and problem solving. A computer session in Fourier analysis using CUPS programs is included in the first course on waves and optics.

### **2.2.1 Mechanics**

CUPS programs have been used in lectures to illustrate topics on the harmonic oscillator, coupled oscillators, rigid body motion, two-dimensional motion with velocity dependent friction and two-particle collisions.

MATLAB programs constructed by the teacher have been used to illustrate the effect of inertial forces in rotating reference systems, Kepler motion, the motion of particles in different types of central force fields, the chaotic behaviour of the double pendulum and two-particle scattering at relativistic energies.

Advanced problems, requiring a few days work, have been given to students to solve with help of computer. Typical such problems are motion of charged particles in cylindrically symmetric electric fields, coupled oscillators, anharmonic oscillators, determination of principal axes and principal moments of inertia for polyatomic molecules with a given geometry. These types of problems lead to differential equations, systems of differential equations, non-elementary integrals and eigenvalue problems which can be solved with the numerical routines in MATLAB.

### **2.2.2 Waves and Optics**

CUPS programs have been extensively used in lectures to illustrate electromagnetic waves, different states of polarisation, refraction and diffraction, the Michelson interferometer and the formation of the rainbow.

The students use MATLAB to solve problems involving Fourier analysis using the powerful FFT routine in MATLAB. Typical such problems can involve frequency analysis of a complicated signal and transforming the interferogram from a Fourier transform spectrometer into a spectrum.

### 3 Courses in Quantum Mechanics

#### 3.1 Quantum Mechanics for Physicists

The CUPS programs in Quantum Mechanics (QM) were introduced into the introductory course in Quantum Physics given during the fifth semester of the Physics studies. The course was defined by the book "Quantum mechanics" by Sara M. McMurry [4] and covers the normal topics of a first course in quantum mechanics. The course was taught through traditional main lectures involving all students combined with separate demonstrations and discussion sessions lead by the main lecturer and involving half the students each time. This was complemented by exercise sessions once a week and also tutorial sessions involving smaller groups of students and lead by highly qualified assistants (PhD students, senior lecturers and professors) from the regular staff. The computer programs were mainly used during the lecture and half-group sessions either as planned demonstrations or as illustrative tools, replacing the traditional blackboard, during class or during discussions at the breaks between lectures.

Quantum mechanics introduces an additional level of conceptual complexity compared with the classical physics courses in that there is very little previous "every-day-experience" that the students can relate to. The simultaneous introduction of new physical and philosophical concepts (probability amplitudes, indeterminacies, quantization etc) and the mathematical tools to describe these (Hilbert space, general orthogonal function sets, alternative representations) make a substantial fraction of the students initially lose perception of the physical contents. For many of these students it takes too long to build up a picture of the processes described by means of QM and it becomes a serious impediment to their studies. Here illustrations and model experiments performed on the computer have an important function in bridging this gap and in quickly providing an intuitive feeling for the properties of the solutions.

The CUPS programs provide a simple way to construct or modify a rather general potential and to solve the Schrödinger equation for this potential and display the results. It is not only easier, but also more instructive to use the computer for this purpose. The computer screen was projected onto the wall by means of an overhead display.

The QM part of the CUPS system consists of a number of different programs covering diverse aspects of quantum mechanics. The programs that were employed in the teaching were Bound1d, Latceld, Qmtime and Scattr1d, which all treat the one-dimensional Schrödinger equation. These one-dimensional programs were very simple to use and gave very clear pictures of the physical situation, while the three-dimensional counterparts (Bound3d and Scattr3d) seemed to require more effort. The program Bound1d, in particular, provides the possibility to solve for eigenvalues, eigenfunctions and probabilities for quite general potentials. In addition it is possible to use the integration routines to evaluate the expectation values or transition properties based on the obtained eigenfunctions. This was extensively used to illustrate bound states, quantization, tunneling, orthogonality and superposition of eigenstates. The Latceld program

extends the allowed potentials towards periodical systems and shows the build-up of band structures. The possibility to manipulate the individual wells was used to illustrate the effects of doping and impurity levels. Summing up the densities for a half-filled or filled band with an added electrical field shows the difference between a conductor and insulator from this particular aspect. The Qmtime program was used quite a lot to illustrate fundamental concepts, such as spreading of wavepacket, penetration, scattering etc while Scattr1d was used to illustrate the development of scattering and transmission with potential and energy. The conditions on the wavefunction for perfect transmission were done graphically, by showing the wavefunction for cases with perfect transmission or maximum reflection.

The students were repeatedly encouraged to try these programs for themselves, but no formal exercises or hand-ins were required. Several students did, in fact, try the programs on their own. The use of the CUPS programs and the computer improved quite substantially the flexibility in the teaching and added a new dimension to the teaching of the subject. It should be particularly noted that the teacher was quite experienced and had already given the course a number of times, but the advantages were so obvious that there were no difficulties making the transition from blackboard-based to computer-oriented teaching of the subject. The experiences from the pedagogical experiment were transferred to two new courses given in the spring of 1997 where the advantages of illustrative computer demonstrations were found to be even greater. The result was a course in "Computer Chemistry" given at Stockholm University and the theory part of a course on "Catalysis" given at Chalmers Institute of Technology, Gothenburg.

### **3.2 Quantum Mechanics for Chemists (Computer Chemistry)**

This quantum mechanics course for chemists is completely new and comprises 10 weeks given jointly by the departments of physical chemistry, quantum chemistry (within the Department of Physics), biochemistry, biophysics and theoretical chemistry. All departments except that of quantum chemistry are organized within the Faculty of Chemistry. The part given by the physics-based quantum chemistry group corresponded to three weeks of lecturing and our task was to introduce the students (second year chemistry students with no mathematical or quantum mechanics background) to quantum mechanics and quantum chemistry. The challenge to discuss the consequences of the Schrödinger equation and its application to problems in chemistry with such little time available and to such a mathematically unprepared group of students was very successfully solved using the computer. This allowed a discussion of the models and of the properties of the solutions while avoiding the tedious and, for this group of students, irrelevant specific solution of the equations. This approach was very much appreciated by the students. Since no teaching material was available supporting this particular approach to quantum mechanics for chemists, focussing on the qualitative aspects still using a completely correct construction of the equations, it was felt that a pedagogical material should also be developed. This resulted in a 62-page compendium where the

models including much of the mathematics were set up. The equations were discussed from a qualitative point of view, but the actual solutions were performed on the computer. For the initial teaching of quantum mechanics, the CUPS program on Quantum Mechanics was extensively used. This made the teaching quite simple since concepts such as the uncertainty principle, interference, quantization, barrier penetration and probabilities could be easily illustrated in a way that the students could relate to. The second part of the course allotted to the quantum chemistry group was taught based on the MacSpartan program [5], where the molecular Schrödinger equation is set up and solved at different levels of approximation. This is where the chemistry was introduced, with structure optimizations, illustrations of vibrational modes in a molecule and molecular orbital theory. The interpretations i.e. probability amplitudes, character of wave functions (number of nodes, energy level spacing) probabilities etc, were carried over from the CUPS program teaching. The CUPS program was actually used in combination with MacSpartan to repeat and underline special concepts. Five computer experiments on topics such as stabilization of amino acid zwitterions in solution, heat of formation of several species, were done as obligatory lab work for the students. These were very much appreciated and underlined the importance in selecting the appropriate software. A common comment from the students was that the menu-oriented set-up of the MacSpartan program allowed them to focus on the chemistry content in doing the experiments on the computer. In comparison, certain other parts of the course used more complicated programs that implied for the students an inordinate amount of time spent on understanding how the input should be done. The simultaneous use of both PC-based (CUPS) and Macintosh based (MacSpartan) software implied the additional complication of having to handle the switching back and forth between the two environments in the lecture hall while lecturing.

With the availability of the MacSpartan software the experiment to change the way of teaching the theory to technology students of the Chemical Technology department was also done. In previous years the course had been taught using overheads, blackboard and videos. One of the main aims was to make the students appreciate the fact that theoretical calculations are beginning to make an impact also in the Technology environment (process and catalyst design) that they will be working in. The videopart shows Scanning Tunneling Microscope pictures of motion of molecules on a substrate in real time to illustrate the molecular control that is now possible and also a session using the UNICHEM [6] program package. This package has a functionality and layout similar to that of MacSpartan and this part was replaced by an interactive session. It was clear that several fundamental concepts were lacking in the students' background and much of the prepared lecture had to be replaced by a session using MacSpartan, where one could easily build up the concepts and discuss them with the students. This also had the very important result that the students realised the ease with which one could perform the calculations and thus quickly get to the important points. Since the aim of the lectures was really to introduce theoretical calculations to the students and to make them open to the

concept, it was probably the best way to get the concept across. The students were very favorable to this part of the course on Catalysis.

In summary, the most important contributions to the teaching from the use of these computer programs has been the flexibility to set up models and to solve them interactively in a discussion form with the students. The computer program brings forward the contents of the solution while eliminating the mathematical intricacies, which can be discussed much more easily at a later stage when the students know and have grasped what it will lead to. For teaching quantum mechanics and quantum chemistry to chemists this has been absolutely essential, but it is clear that also for the physics students the simultaneous introduction of concepts of quantum mechanics and "new mathematics" (Hilbert space, orthogonal functions, expansion of the wave function in eigenstates, expectation values etc) often leads to a period of difficulty. Illustrating the concepts in graphical form on the screen is a great help in overcoming these difficulties.

#### **4 Alternative Examination Forms**

We have started to introduce alternative examination forms. Computer program packages like CUPS and MATLAB have been used in special obligatory laboratory and project works. In the mechanics course the solving of more intricate numerical problems using MATLAB has been part of the examination. These attempts have worked very well and will be extended in the future.

#### **5 Summary**

We have successfully implemented the use of teaching packages like CUPS programs and MATLAB in several of our existing physics courses. An important part of the work has been the critical study of existing material and selection of the parts that fit in the existing courses.

A new course in "computer chemistry" was developed where the use of computers was introduced from the very beginning in a systematic way. The computers were also used for obligatory laboratory work.

The most important contributions to the teaching from the use of these computer programs has been the flexibility to set up models and to solve them interactively in a discussion form with the students. The computer program brings forward the contents of the solution while eliminating the mathematical intricacies, which can be learned at a later, more appropriate time.

The implementation of new teaching methods will lead to alternative examination forms where the computer will be a natural tool. Our attempts to use the program packages in special project works demonstrate an attractive alternative examination form.



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### References

1. FLIP Collaboration: I. Cohen<sup>1</sup>, G. Edvinsson<sup>2</sup>, G. Karlsson<sup>1</sup>, C. Johannesson<sup>3</sup>, K. E. Johansson<sup>2</sup>, S. Nilsson<sup>2</sup> and L.G.M. Pettersson<sup>2</sup>  
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2. CUPS guides, <http://www.wiley.com/Guides/Physics/CUPS.html>  
For a review see also <http://www.ph.surrey.ac.uk/cti/cups/review.html>
3. MATLAB is a registered trademark, Math Works, Inc.,  
<http://www.mathworks.com>
4. Quantum Mechanics, Sara M. Mc Murry, Addison-Wesley 1993
5. MacSpartan, registered trademark,  
<http://www.wavefun.com/software/desktop/mphome.html>
6. UNICHEM, <http://www.oxmol.com/prods/unichem/cap>