Teaching thermodynamics using algorithms. The correlation between programming and physics

Enseñanza de termodinámica con algoritmos. Correlación entre la programación y la física

SARANTOS PSYCHARIS

Greek Pedagogical Institute, Department of Pedagogy, University of Aegean, Athens, Greece
psycharis@Rhodes.Aegean.gr

Abstract

In the context of the relation of entropy with the number of microstates, we developed a source code in C++, for the distribution of a definite number of quanta among the atoms of a solid. This application can be used by grade 12 students and first year university students studying physics, in the framework of the course in thermodynamics, for understanding the relationship between entropy and the number of microstates. This application has been used in the context of teaching algorithms and was implemented at a private institution in preparing students to enter Greek Universities. The aim of this project is to help visualize key issues about entropy and the number of microstates and to examine the attitude of students against the theory of algorithms when the teaching of algorithms is connected with other disciplines.

Key words: *teaching thermodynamics, entropy, programming, algorithm, quanta.*

Resumen

En el contexto de la relación de la entropía con el número de microestados, se desarrolla el código en C++, para la distribución de un número entre los átomos de un sólido. Esta aplicación puede ser usada por estudiantes de grado 12 y estudiantes de universidad de primer año que estudian física, en el curso de termodinámica, para comprender la relación entre la entropía y el número de microestados. Esta aplicación ha sido usada en el contexto de los algoritmos de enseñanza y fue implementado en una institución que prepara a estudiantes que entran a universidades griegas. El objetivo de este proyecto es ayudar a visualizar los asuntos clave sobre la entropía y el número de microestados y revisar la actitud de los estudiantes en la teoría de los algoritmos cuando la enseñanza de los algoritmos está relacionada con otras disciplinas.

Palabras clave: *enseñar termodinámica, entropía, programación, algoritmo.*

INTRODUCTION

The impact of the new technology in education is especially strong in Natural Sciences. Modeling and computer aided experiments can give deeper insight into the nature of physical phenomena and bring the real world into the science lessons (BORKOWSKI, 2002). In contrast with the process of acquiring factual knowledge from textbooks, ICT (Information and Communication Technologies) facilitates the scientific exploration of physical reality. ICT can be incorporated in classroom through the: integration of ICT in subject content, the integration of experimental and model approaches and the integration of different science disciplines. Computer simulation has put a new whole spin on science education reform act, redefining also the role of teachers and reshaping the classroom learning experience. The use of computer simulation tasks to enhance learning in the science classroom, either before or after completion of a didactic unit of instruction, has become the focus of most recent research studies (AKPAN, 2001).

THOMAS and HOOPER (THOMAS and HOOPER, 1991) describe a simulation as a computer program containing a manipulability model of a real or theoretical system. The program enables the students to change the model from a given state to a specified goal state by directing it through a number of intermediate states.

THE FORBIDDEN AND THE SPONTANEOUS PROCESSES

It is considered that the second law of thermodynamics expresses the most dynamic and general idea of Physics. This law states that: Any process whose sole effect is the conversion of heat to work is impossible. Using this law we can explain the creation of cyclones, the decay of snowmen, the necessity for repair of the houses. The fact that we have never seen drops of water at room temperature to transform to ice cubes, perfumes to enter spontaneously to the small nice jars, broken glasses to rejoin leading to the initial jar is explained in terms of the second law.

The second law can justify why heat does not flow spontaneously from cold objects to hot objects, or why heat can not be converted entirely to work (for example the heat from a steam engine is not converted 100% to the work for the motion of the piston). On the contrary, work can be converted entirely to thermal energy, for example by rubbing our hands together. The consequences of this are that in every process there is a conversion of energy into internal energy. Even light emitted from the stars as thermal radiation, has not been observed as re-emitted radiation from our eyes. Stars die when their nuclear fuel is consumed, while the consumed fuel is not reproduced in the same quantity, so the number of produced stars is less than that of the initial ones (DAVIES, 1983).

The verification of the second law is also realized in the case of the human life, where people are born, grow up and finally die, while the reverse process has never been observed. The reverse of the above processes are allowed from the first thermodynamic law, which is a generalized form of the conservation of energy, but are forbidden by the second thermodynamic law.

A natural path to start understanding the second law is by thinking of the direction of flow of energy in every process. All the different forms of energy have the tendency to diffuse, leaving the total amount of energy constant, while a certain amount of energy has appeared —inevitably— in the form of heat energy: Cars (when their kinetic energy is reduced by friction after releasing the throttle), people (burning the calories of chemical energy), power stations, air in the tires, sound waves are all examples of the transformation of organized energy to heat. Consequently, another statement, which expresses the Second law, would be: energy has the tendency to flow from a point where it is concentrated, becoming dispersed.

There are certain processes where the diffusion of energy (i.e. sound waves) is quite obvious and cannot be hindered from occurring, but there are some others where diffusion does not happen right away. The organized form of gravitational potential energy (suppose we keep a stone in our hands) is not diffused to the surrounding, but it has the tendency to diffuse immediately after we release the stone. This temporary forbiddance of the Second Law may be the reason for our existence in the world and justify the infrastructure we observe.

ENTROPY-DISORDER-PROBABILITY

Another statement for the second law is: As time passes, for every closed system, the entropy increases. The word entropy was created by CLAUSIUS (CLAUSIUS, 1864) and is made up of the word "tropy", which means transformation, while "*en*" means the energy-taking place in thermodynamics. The entropy of a system is a characteristic property of the system, and for its better understanding we have to deal with the microscopic scale. BOLTZMANN, using the molecular properties of a system invented the connection of the macroscopic meaning of entropy with the microstates of a system. BOLTZMANN'S idea was that the macroscopic description of a system is not complete, since when the system is in a certain macro state, it is possible to be in one of many available microstates. The physical quantity that allows the counting of different microstates, which correspond to the same macro state, is the entropy.

In the atomic scale, there is time reversal symmetry, resulting in time-reversal equations of motion and the exclusion of a final microscopic equilibrium state. On the other hand macroscopic systems are not time reversed and lead to a final equilibrium state. Therefore the problem was to find the connection between the microscopic and the macroscopic level. BOLTZMANN using the concepts of molecular chaos and incorporating the theory of probability into the laws of mechanics, proposed the solution. The result was an equation for the time evolution of the system, which was not time reversible, and had its origins on the assumption of the molecular chaos. When a warm and a cold body are in contact, there is a greater possibility that energy flows from the warmer towards the colder one, because in the warmer body there are more energy quanta.

When a stone hits the ground, a part of its organized Kinetic Energy is rearranged between the particles constituting the stone, leading the molecules in random motions (heat). The reverse procedure, during which the random motions of the molecules will lead to an organized motion, with molecules having parallel speeds, is equivalent to the transformation of heat to work and has very small probability to occur. When the system is in a disorder, its energy is randomly allocated between the particles of the system in many more ways than when allocated in a single manner. Entropy is connected to disorder and expresses the number of possible ways in which the energy of a system is allocated between its constituting particles.

NUMBER OF MICROSTATES AND ENTROPY

The correlation of entropy with the number of possible microstates can offer a deeper insight on the explanation of the appearance of some processes against some others. When we deal with a large number of particles, which behave in a random way, we use the Probability Theory, considering all the possible states of the system to have the same possibility. The entropy (macroscopic quantity) is connected to the microscopic level through the relationship S=K.lnW, where W is the number of symmetric (non distinguishable microstates), which leave invariant the macroscopic state of the system. In the final state of the system the total entropy (equivalently, the disorder) will have reached its final value. Under these considerations BOLTZMANN correlated the entropy of a system with the probability that it is led to disorder.

A simple example for the understanding of the maximization of the number of microstates in the equilibrium state is the following:

We can consider the distribution of certain quantum of energy between the atoms of a solid body. Due to the random interactions among the atoms, the total energy remains constant but the number of ways in which it is distributed between the atoms differ (assuming that the number of energy quanta of an atom, is independent of the number of quanta in its neighboring atoms; this is a model proposed by EINSTEIN).

There are combinations, which occur more often and in the state of equilibrium and there is a combination, which corresponds to the greatest number of possible microstates.

Suppose that the total number of atoms is N and the number of quanta is Q.

We plot the following cases.

Case 1: N=6 and Q=4, Q=5, Q=6, Q=7, Q=8, Q=9, Q=10, Q=11

Case 2: N=7 and Q=4, Q=5, Q=6, Q=7, Q=8, Q=9, Q=10, Q=11

The macro states and the microstates are presented only in the case N=6,Q=9 – while the rest can be studied in the same way. For a better understanding we present the source code for the case N=7.

P(0), P(1) etc. correspond to the average number of particles in the zero state of energy, first state of energy and so on.

From Mathematics it is known that there exist $\frac{(N+Q-1)!}{Q!(N-1)!}$ (1)

ways to distribute the Q quanta between the N oscillators.

This relation is verified in all cases but it is not used to produce the results (that is why we use the term experimental proof of the BOLTZMANN'S distribution).

We also present two graphs -using Microsoft Excel – of P(i) as a function of the energy(i=1,2,..).

To calculate P(i) we used the relation: $P(i)=\sum_{k=1}^{macro} n_{ki}P_k$, where macro represents the number of macrostates and P_k is the number of microstates of the k – macrostate divided by the total number of microstates.

For the case N=6, Q=9, macro=26 (as it is presented below) and the number of microstates is 2002 (as it is verified easily from the formula (1))

For that case $P(0)=\sum_{k=1}^{26} n_{k0}P_k$

Where, $P_1=\frac{6}{2002}$, $P_2=\frac{30}{2002}$, etc.

and $n_{10}=5, n_{20}=4$ etc.

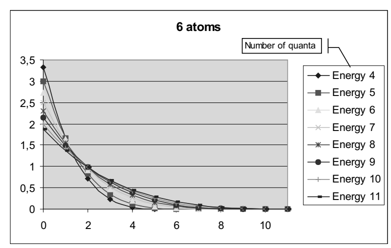
We developed a program in C++ which simulates an experiment for the verification of the BOLTZMANN'S law, in the framework of teaching the concept of entropy to high school students. The program displays the following results. In the last column of the table, named macro-solutions, we present the number of microstates for every macrostate.

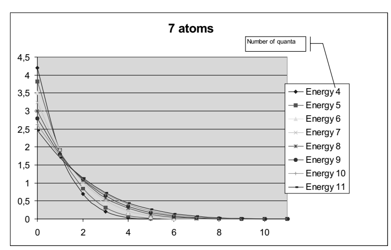
Macro solutions

5 0 0 0 0 0 0 0 0 1 6
4 1 0 0 0 0 0 0 1 0 30
4 0 1 0 0 0 0 1 0 0 30
4 0 0 1 0 0 1 0 0 0 30
4 0 0 0 1 1 0 0 0 0 30
3 2 0 0 0 0 0 1 0 0 60
3 1 1 0 0 0 1 0 0 0 120
3 1 0 1 0 1 0 0 0 0 120
3 1 0 0 2 0 0 0 0 0 60
3 0 2 0 0 1 0 0 0 0 60
3 0 1 1 1 0 0 0 0 0 120
3 0 0 3 0 0 0 0 0 0 20
2 3 0 0 0 0 1 0 0 0 60
2 2 1 0 0 1 0 0 0 0 180
2 2 0 1 1 0 0 0 0 0 180
2 1 2 0 1 0 0 0 0 0 180
2 1 1 2 0 0 0 0 0 0 180
2 0 3 1 0 0 0 0 0 0 60
1 4 0 0 0 1 0 0 0 0 30
1 3 1 0 1 0 0 0 0 0 120
1 3 0 2 0 0 0 0 0 0 60
1 2 2 1 0 0 0 0 0 0 180
1 1 4 0 0 0 0 0 0 0 30
0 5 0 0 1 0 0 0 0 0 6
0 4 1 1 0 0 0 0 0 0 30
0 3 3 0 0 0 0 0 0 0 20

P(0)=2.14286
P(1)=1.48352
P(2)=0.989011
P(3)=0.629371
P(4)=0.377622
P(5)=0.20979
P(6)=0.104895
P(7)=0.044955
P(8)=0.014985
P(9)=0.002997
Macro = 26.
Micro = 2002.

Excel Graphs: Findings -Probability versus Energy





METHODOLOGY

This investigation contained two aims:

The first was to show students that ICT can and should be applied to the natural sciences so as to be able to comprehend concepts better and easier as well as to engage in a visual representation of key concepts.

However, our main aim was to use the algorithm for the discipline called "developing ICT applications using algorithms".

Usually, students studying this subject mainly focus on ICT related problems and not on their connection with other disciplines taught in class. As a result, first-year undergraduates studying engineering, physics etc are confused and seek some advice on the relevance of ICT in a pragmatic situation relating to their chosen subject.

Consequently, it was decided that such an application could be implemented in thermodynamics, for example, and directly linked to the concept of entropy which may not form part of the syllabus itself, but may be familiar to the student from the press etc. In an attempt to materialize this programmer, students were asked in their first meeting, to read chosen articles which were given to them in advance. The sample size was 25 students. Following the second meeting, students showed an increased interest in topics such as states of disorder, increase in entropy, thermal death) etc. It is worth noting that in the meeting, both the physics and IT instructors were present. After the necessary clarification of terms and concepts, students were prompted to create an algorithm for the microstates of a given energy distribution. The response was very encouraging; 21 out of the 25 volunteered to create a pseudo code. This process required two additional sessions, the first for further discussion and clarification of key points and the second for the announcement of the individual results. The added value of this practice was the opportunity for students to express a strong will to continue to contextualize most, if not all, given problems.

Another important change which was noticeable was the immediate positive impression that this subject created to students and the enthusiasm it generated. Note that for students who intend to study Computing at University, this is a compulsory subject. It is also compulsory for students who intend to study engineering, mathematics, physics, economics etc.

Prior to this implementation, the great majority of students (95%) wishing to study Computing believed that this lesson was useful, while only 60% of students who do not intend to study Computing, found this lesson useful. This percentage dramatically increased to 97% immediately after the exposure to this lesson. In addition, students expressed that it would be preferable to expose them to such lessons in both physics and mathematics, before they are taught in the conventional way.

CONCLUSIONS

In the framework of teaching the concept of entropy to high school students, we constructed a simulation program to experimentally verify the BOLTZMANN's Law. At some stages, students with knowledge of programming were involved in the creation of the source code. During the exploration of this work students expressed their willingness to deal with issues like the relation of entropy with the symmetry, the evolution of the universe e.t.c, which gives an indication that this work was quite fascinating for them. Finally, from the graphs there is an "experimental" proof of the BOLTZMANN's Law and as the number of the quanta is increased, the exponential decay is getting less steep. The work includes a lot of logic connected to the creation of algorithms and thus can be extended to upper secondary school curriculum in the context of the creation of algorithms to solve certain problems in different subjects.

The process of programming was made in the laboratories of a private institution for the preparation of Greek students to enter Greek Universities.

Students were willing to create the source code .The purpose of this process is the comprehension of the linkage between algorithmic methods and simulation of physics phenomena which will help students comprehend complex physical phenomena as well as develop the necessary computing skills.

BIBLIOGRAPHY

ADAMS, STEVE, "No Way Back", *Nature*, 1-4, October 1994.

AKPAN, J.P. (2001), Issues associated with inserting computer simulations into biology instruction: A Review of the Literature. *Electronic Journal of Science Education*, 5 (3), Available: http://unr.edu/homepage/crowther/ejse/ejsev5n3.html

BORKOWSKI, J. (2002). NEST - New Educational Technology for Science Teachers Training, Proceedings from UNESCO Global Forum on Learning Technology, Learntec Conference Centre, Karlsruhe, Germany.

CLAUSIUS, R., *Abhandlungungen über die mechanische Wärmetheorie*, vol. 1, Braunschweig: F. Vieweg 1864.

DAVIES, PAUL, *God and the New Physics*. J. M. Dent & Sons Ltd 1983.

THOMAS, R. & HOOPER, E., Simulation: An opportunity we are missing, *Journal of Research on Computing in Education*, 23(4), 497-513, 1991.

APPENDIX

Source Code

```
#include <iostream.h>
#define BALLS 7
#define ENERGY 11
#define TOTAL 10
#define MAXMIKRO 9000
#define MAXMAKRO 200
int main()
{
int mikro=0;
int makro=1;
int match;
char end;
int    a[ENERGY][MAXMIKRO];
int    sol[ENERGY][MAXMAKRO];
cout << "Starting testing...";
for (int i1=0;i1<ENERGY;i1++)
{
for (int i2=0;i2<ENERGY;i2++)
{
for (int i3=0;i3<ENERGY;i3++)
{
for (int i4=0;i4<ENERGY;i4++)
{
for (int i5=0;i5<ENERGY;i5++)
{
for (int i6=0;i6<ENERGY;i6++)
{
for (int i7=0;i7<ENERGY;i7++)
{
if   (i1+i2+i3+i4+i5+i6+i7==TOTAL)
{
mikro++;
cout << "Mikro = " << mikro << "\n";
for (int i=0;i<ENERGY;i++) a[i][mikro-1]=0; // midenika ta stoixeia tou
pinaka a
for (int i=0;i<ENERGY;i++)
{
if (i1 == i ) (a[i][mikro-1])++;
if (i2 == i ) (a[i][mikro-1])++;
if (i3 == i ) (a[i][mikro-1])++;
if (i4 == i ) (a[i][mikro-1])++;
if (i5 == i ) (a[i][mikro-1])++;
if (i6 == i ) (a[i][mikro-1])++;
if (i7 == i ) (a[i][mikro-1])++;
        cout << a[i][mikro-1] << " ";
}
        cout << "\n";
}
}}}}}}
for (int j=0;j<ENERGY;j++)
        sol[j][0] = a[j][0];        // midenika ta stoixeia tou pinaka sol

for (int k=1;k<mikro;k++)
        {
        match=0;
        for (int j1=0;j1<makro;j1++)
        {
        if
((a[0][k]==sol[0][j1])&&(a[1][k]==sol[1][j1])&&(a[2][k]==sol[2][j1])&&(a[3][k]==sol[3][j1])&
&(a[4][k]==sol[4][j1])&&(a[5][k]==sol[5][j1])&&(a[6][k]==sol[6][j1])&&(a[7][k]
==sol[7][j1])&&(a[8][k]==sol[8][j1])&&(a[9][k]==sol[9][j1])&&(a[10][k]==sol[10][j1]))
        {
        match++;
        }
        }
        if (match==0) {
        for (int s=0;s<ENERGY;s++)
        sol[s][makro]=a[s][k];
        makro++;
        }
   }
        cout << "\n" <<"MAKRO SOLUTIONS \n" ;
        for (int k1=0;k1<makro;k1++)
        {
        for (int k2=0;k2<ENERGY;k2++)
        cout << sol[k2][k1] << " ";
        cout << "\n" ;
        }
        cout << "Makro = "<< makro <<".\n" ;
        cout << "Mikro = " << mikro << ".\n";
   cin >> end;
   return 0;
   }
```


Received: 23.10.2004 / Approved: 9.09.2005