

Book Review

Consortium of Upper-level Physics Software (CUPS)

Thermal and Statistical Physics Simulations

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156 pages

The Consortium of Upper-level Physics Software (CUPS) is an international group of 27 physicists who are developing simulations for physics students and their instructors. This book including the associated computer programs is the eighth in a CUPS series that covers many important fields of physics.

In accordance with the aim of the CUPS project, this 'book' is not a book in the traditional sense: it is a manual for the associated programs and a brief introduction to the physics involved. The book and the programs are almost unusable without each other. The word simulation in the title means programs with graphics and movies to assist the understanding of some otherwise difficult physical theories and phenomena. With the help of the programs the interested reader is able to 'touch' a physical theory, to experiment with different situations. The source code of the (Pascal) programs is included, so everybody can change and supplement the simulations with more details on the physics and the numerical methods.

The book describes seven program groups dealing with different topics of equilibrium phenomenological and statistical theories.

The Introduction contains a brief description of all the CUPS programs in the whole series, so the reader interested in other subjects of physics can find a detailed description.

Following the introduction, the first chapter 'Thermodynamics of Fluids' helps to understand the phase diagrams of two real gases: the water and the Van der Waals gas. Here one can study first-order phase transitions in different phase diagrams, drawing equilibrium phase curves in one diagram and see how this path looks in the other phase diagrams. The user can also extract all important thermodynamic data at any point in a phase diagram. The book explains how the program uses the corresponding physics and the essence of the physical theory behind that.

The second chapter deals with different 'Engines'. We can design our own engine (closed equilibrium phase curve) with specific processes, and the program

computes the thermodynamic properties of the engine (work done and the heat exchanged for each process and the efficiency of the engine, etc.). Moreover, simulations of the Diesel, Otto and Wankel combustion engines are also presented. The third chapter gives an 'Introduction to Probability and Statistics'. Different little programs simulate the Galton board (demonstrating the binomial and normal distributions), the radioactive decay of atoms (demonstrating the Poisson and exponential distribution), the two dimensional random walk (joint probability, etc.). Additionally, the example of the Kac ring illustrates some aspects of the statistical and exact mechanical descriptions, and another example is given of the origin of the chaotic motion, where we can see how the close paths diverge in a stadium like billiard.

The fifth chapter 'Statistical Properties of Gases, Liquids, and Solids' contains a molecular dynamic simulation of a collection of particles with given interaction (hard disc model and Lenard-Jones potential is the default). Various thermodynamic phenomena can be displayed with the help of this simulation and one can form an idea of the statistical notions and models.

The sixth chapter deals with 'Quantum Ideal Gas'-es. Here the behaviour of the ideal Fermi, Bose and Boltzman gas can be studied and some distribution functions and thermodynamic properties are calculated and plotted.

The seventh chapter 'The Ising Model and Critical Phenomena' is written on the important (and popular) problem of the critical phenomena with the example of the Ising model. Here all the basic notions of the subject (critical exponents, scaling, renormalization group method) are more or less explained in the book and illustrated in the program. The program uses different types of Monte Carlo algorithms to give the quasidynamics of the model with different thermodynamic properties (constant energy, heat bath, etc.).

The last chapter of the book gives a brief overview on the use of the programs for those who are not interested in the physics and other details.

Each chapter contains exercises, that call the attention of the reader to different physical phenomena in the programs, and some suggestions for the possible modification of the source code to make bigger alterations and additions.

I think that the programs and the book are good examples of the use and the benefit of computers in teaching and studying physics. We can really touch the theoretical models, the visualisation helps us to understand the phenomena and to grab the essence of the subject. Moreover, the game with the source code, the possible additions can give us an idea of the trial and error properties of scientific programming.

Unfortunately, the theoretical descriptions are sometimes oversimplified. For example on page 25 we can read about thermodynamic potentials that 'The difference between the various potentials is that they are functions of different variables.' Another example is on page 61 where the text is about the Recurrence theorem of Poincaré and the book states that Zermelo's objections against the H theorem (based on the recurrence) 'is important only for fundamental reasons, not realistic systems.' We should realize that the entropy of a

system whose dynamics are governed by Hamilton's equations, or any set of differential equations for that matter, cannot change. This result is independent of the size of the system and the recurrence theorem, too. The problem is that just because the points of the phase space of a mechanical system are recurrent, densities need not be, and indeed we can give a necessary and sufficient condition for the entropy of a system do increase to its maximum, which is completely compatible with the Poincaré recurrence theorem (see M. C. Mackey: *Time's Arrow: The Origin of Thermodynamic Behavior*, Springer 1992). So some refinement of that kind of statements would be reasonable.

Another reservation is that the titles of the chapters are sometimes misleading, we expect for example that such an ambitious title as 'Thermodynamics of Fluids' covers more on this subject. An important improvement would be to see not only the thermostatics but the real dynamics of this kind of simple systems. This addition would improve the 'Engines' part, too. In general, the book deals with simulations in thermostatics and equilibrium statistical physics. Consideration and treatment of non-equilibrium thermodynamics or at least the real dynamical properties of the treated systems would improve significantly the understanding of the physics involved.

We can recommend the book (and the programs) to those who are studying or teaching thermal or statistical physics at the university level. The book may be of help in the understanding of these subjects, giving an 'experimental background' for the interested reader.

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