AC 2007-747: ON REMOTE AND VIRTUAL EXPERIMENTS IN ELEARNING IN STATISTICAL MECHANICS AND THERMODYNAMICS

Sabina Jeschke, University of Stuttgart

Since 2005, Sabina Jeschke has been associate professor for "New Media in Mathematics and Natural Sciences" and director of the MuLF Center (Multimedia Center for New Media in Education and Research) at TU Berlin. Starting in 2001, her Berlin group has been a driving force behind the development of multimedia technologies at the university, implementing multimedia educational elements in the education of undergraduate students, in particular for engineering students. In 2000 and 2001, she worked as an assistant professor at the GaTech (Georgia Institute of Technology, Atlanta). In May 2007, Prof. Dr. Sabina Jeschke took over a full professorship for "Information Technology Services" at the Universität Stuttgart. Additionally, she acts as scientific and executive director (CEO) of the "Center of Information Technologies" of the Universität Stuttgart. The research of S. Jeschke is aimed at developing new concepts of service-oriented architectures for eLearning and eScience in particular in the fields of mathematics, natural sciences and engineering. She focuses on development and networking of interactive mathematical objects and remote/virtual experiments, on mechanisms for the creation, modification and storage of data in cooperative virtual knowledge spaces, and on the design of intelligent data analysis and validation schemes.

Olivier Pfeiffer, Technische Universitat Berlin

Olivier Pfeiffer received his M.Sc. in Mathematics at the Berlin University of Technology in 2002. His thesis in numerical mathematics investigated “Error Control using Adaptive Methods for Elliptic Control Problems in Matlab”. He has been working in several eLearning projects at the Berlin University of Technology, beginning as a student assistant in the Mumie project - a platform using new pedagogical concepts to support teaching of mathematics for mathematicians, engineers and natural scientists - at the Berlin University of Technology in 2001, as a research assistant at SFB609 in Dresden from 2002-2004, and is now part of the Team of the MuLF-Centre (Multimedia Center for eLearning, eTeaching & eResearch at the TU Berlin). In the past two years, Olivier Pfeiffer focused on the organization and coordination of the involved teams and contributed to several other eLTR related projects. He is also involved in the planning and application of future eLTR projects at the Berlin University of Technology. His research interest focuses on the development of interactive mathematical objects especially supporting the visualization of complex mathematics and physics related problems.

Contact Information:

Technische Universität Berlin

Medienzentrum für Lehre und Forschung

Sekretariat MA 7-2

Olivier Pfeiffer

Mail: pfeiffer@math.tu-berlin.de

Phone: +49/(0)30/314 24603

Fax: +49/(0)30/314 24413

WWW: http://www.math.tu-berlin.de/~pfeiffer

Thomas Richter, Technische Universitat Berlin

Harald Scheel, Technische Universitat Berlin

Christian Thomsen, Technische Universitat Berlin

On Remote and Virtual Experiments in eLearning in Statistical Mechanics and Thermodynamics

Abstract

The science of physics is built on theories and models as well as on experiments. Theories and models structure relations and simplify reality to such a degree that predictions on physical phenomena can be derived by means of mathematics. Experiments allow to verify — or falsify — those predictions. Computer sciences allow a new access to this relationship which is especially well-suited for education. New Media and New Technologies provide simulations for the model, virtual instruments for running and evaluating real experiments and mathematical toolkits to solve equations derived from the theory analytically and to compare the outcome of all three methods. We will demonstrate this approach on two examples: Ferromagnetism and elementary thermodynamics.

I. Introduction

One of the intellectual challenges when learning physics is to understand the roles of a physical theory, a physical model and that of an experiment. These terms are often intermixed and the classical curriculum offering separate lectures for theoretical and experimental physics does not make it easier for students to really comprehend their inter-relation.

Modern eLearning technology may act as a bridge as computer systems make real experiments available over the Internet any time, anywhere, and — even more important — make the measured data electronically available for further analysis. On the other hand, a model for an experiment can be implemented as a simulation within a virtual laboratory making the same physical quantities available for measurement as in the "real" experiment. It makes it easier for a student to compare the outcome of the two approaches and to compare them again with an analytic result of a physical theory. Thereby, similarities and differences between the theory, the model and the experiment can be demonstrated and analyzed.

In this paper, we discuss two important physical systems: first, the physics of ferromagnetism and the Ising model[1] as the most prominent system of statistical mechanics. Second, the physics of ideal gases and -as the corresponding theoretical model- the lattice gas model[2,3] to discuss the concept of entropy phenomenologically as well as statistical thermodynamics.

II. A brief Introduction to the Physics of Magnetism

Materials react differently to an applied external magnetic field; they are either diamagnetic, paramagnetic or display effects due to the correlations of magnetic moments in the material, such as ferromagnetism or antiferromagnetism[4,5]. Diamagnetism and paramagnetism are weak and require relatively large external fields to make them visible. Ferromagnetism, however, is apparent for small external fields. Unlike dia- and paramagnetism, it is a many-body phenomenon where the elementary magnets of an otherwise paramagnetic material interact with each other and couple their magnetic moments such that a macroscopic field is generated. The magnetization M of the elementary magnets in the material adds up with the external magnetic field H to the magnetic induction B[5].

Two properties are now interesting about M for ferromagnetic media: first of all, there is no unique relation between H and the induced magnetization M, but M depends on the history of the process. Ferromagnetic materials show a hysteresis and a plot of the magnetization over the magnetic field has a typical double-S shaped form. Second, the ferromagnetic effect vanishes for high temperatures. If the temperature T becomes larger than the Curie-temperature TC, ferromagnetic materials become paramagnetic and the hysteresis vanishes, thus establishing a phase transition similar to the solid-liquid phase transition observed for water when melting.

In the 1920's, Ernst Ising[1] developed a microscopic model to explain ferromagnetic behavior; according to it, ferromagnets consist of elementary magnets called spins, carrying magnetic moments — in the simplest possible model — pointing into one of two possible directions. They interact with their nearest neighbors in such a way that the energy contribution of a spin-spin pair to the total energy is minimal if the two neighboring spins have parallel magnetic moments and maximal if they are antiparallel. Even though Ising's first attempt o show a phase transition in a one-dimensional spin-chain failed, a two-dimensional model did reproduce all macroscopic effects. A rigorous proof of this model was given by Onsager many years later.[6]

III. Magnetism in Virtual Laboratories

The Virtual Laboratory VideoEasel developed at the TU Berlin focuses on the field of statistical physics and statistical mechanics[7,8]. Implementing a freely programmable cellular automaton[9], VideoEasel is capable of simulating various models of statistical mechanics and related fields.

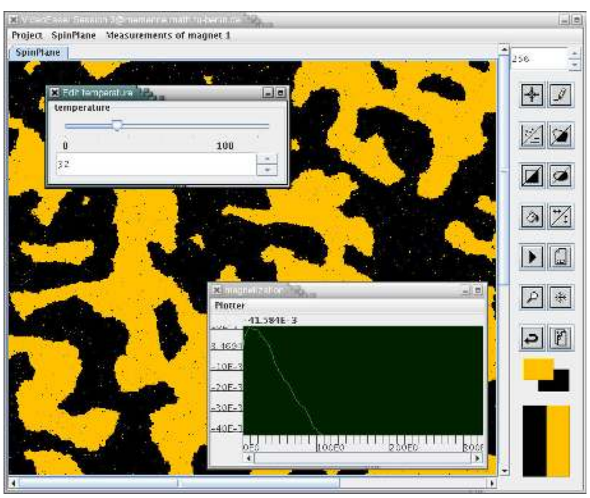

Figure 1. The Ising Model in the virtual laboratory VideoEasel

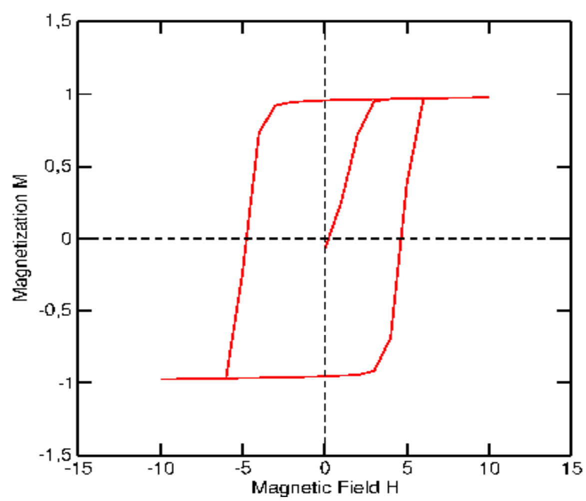

Figure 2. Hysteresis loop of the Ising model for low temperature

Measurements are performed by tools freely plugged into the experiment by the user, allowing to observe magnetization, entropy, free energy or other measuring quantities. When experiments of higher complexity are performed, the experimental results can be automatically exported into computer algebra systems for further analysis. To enhance cooperative work between students or students and their teachers, VideoEasel is able to support distributed measurement processes on the same experimental setup, including remote access from outside the university[7].

In order to investigate the Ising model, VideoEasel implements the Metropolis dynamics[10.] (See Fig. 1). A spins is drawn at random and flipped if either the overall energy of the model decreases after the flip, or the energy can be borrowed from a heat-reservoir. The user is able to control the temperature T and external field H and then measures quantities as the magnetization M. If we plot the relation between M and the field H for low temperature, a hysteresis loop is found. (See Fig. 2). This figure vanishes for high temperatures.

Additionally, our model allows us to measure an additional parameter, namely the Helmholtz Free Energy F.[11] This quantity is phenomenologically defined as the fraction of the overall energy of the model that is available for mechanical work. If we measure M and F -each depending on H- while starting from a random spin configuration, we get the graphs shown in 3. It is now easy for our students to conjecture that M must be proportional to the negative derivate of F with respect to H. After having seen that, our students easily derived this from the Gibbs state of the Ising model[11], and thus our experiment was also didactically successful.

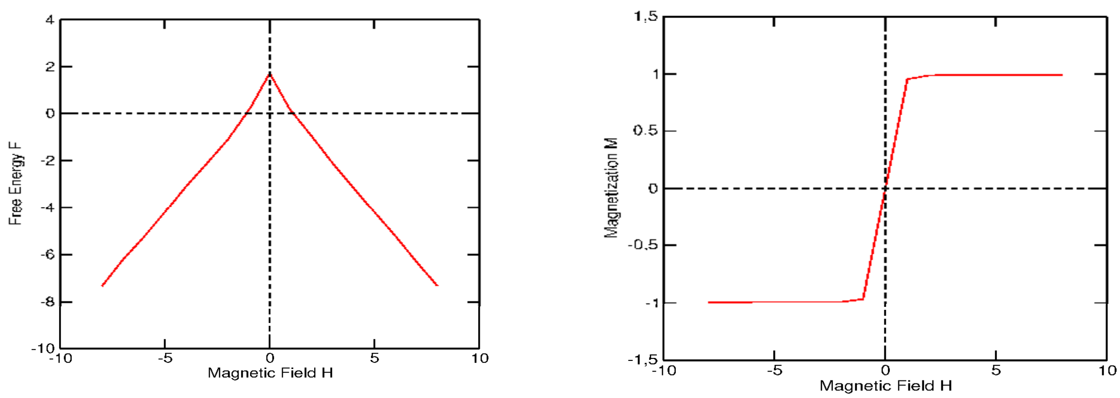

Figure 3. Free energy (top) and magnetization(bottom) as functions of the external field

IV. Investigating Hysteresis in Remote Experiments

Complementary to Virtual Laboratories, Remote Experiments are real experiments remotely controlled by the student from outside the laboratory. A Remote Experiment consists of two vital parts -namely the experiment itself- and a computer interface allowing control over the experiment via Internet. For the latter, we use National Instruments LabView[12], which also provides a convenient web-interface. In order to view and control the experiment, a freely available web browser plug-in has to be downloaded and installed. Remote experiments can easily be combined or extended due to the modular programming structure of LabView.[13]

We can now run the same experiment -namely that of measuring the hysteresis loop of magnetization vs. magnetic field- in reality: a magnetic coil generates a magnetic field H that is proportional to the current passing through it, which is controlled by the computer. The magnetic field magnetizes a ferromagnetic core. The Magnetic induction B is measured by a Hall probe, see Fig. 4. The measured value is then digitized by an analog-digital converter that provides a digital output port and by that made available from the computer system.

V. Virtual Laboratories & Remote Experiments – Similarities and Differences

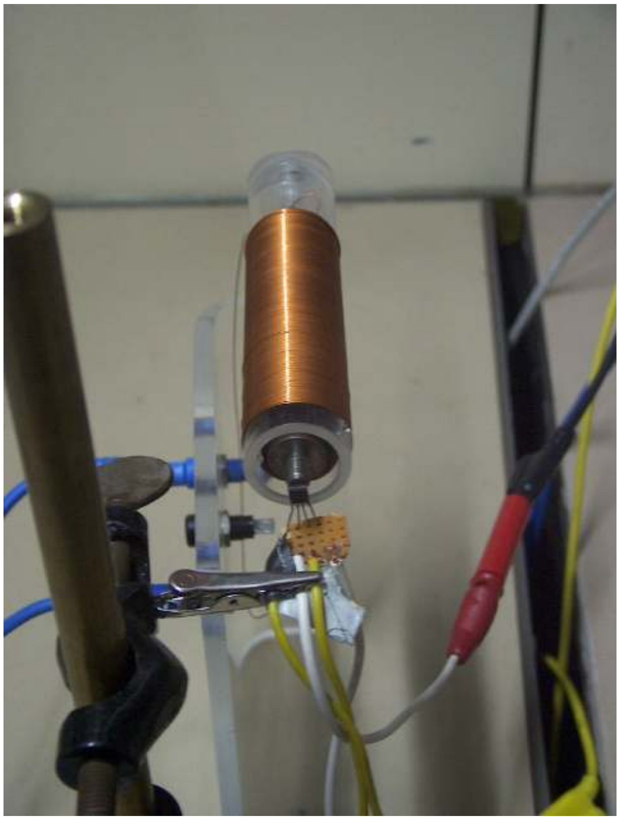

Figure 4. Setup of the remote experiment on hysteresis, the magnetic coil in the middle, Hall probe in front

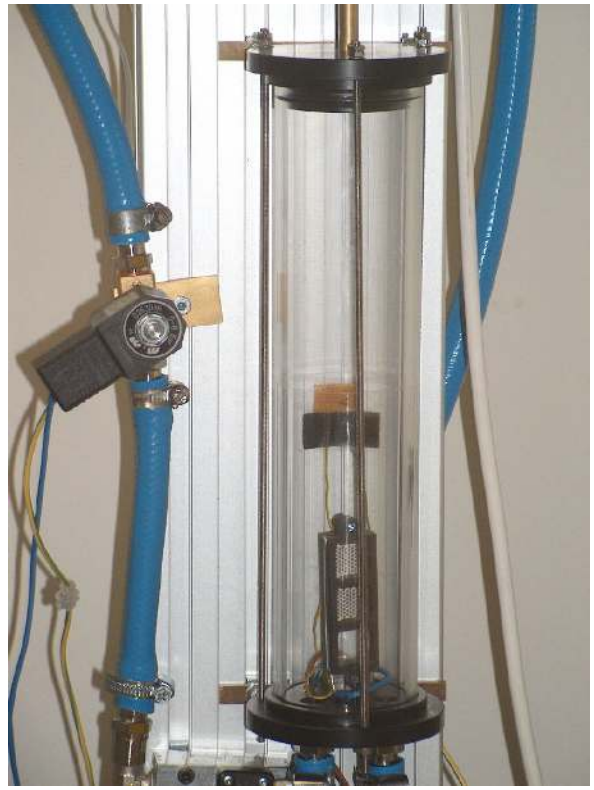

Figure 6. Remote experiment on thermodynamics: a piston (top of the image) controlled by a motor (not shown) compresses gas in a glass cylinder. A temperature and pressure sensor (middle) measures physical observables. A heater (bottom) allows heating the gas volume.

At first glance, both the experiment and the model show the same hysteresis effect: the relation between magnetization and magnetic field cannot be represented by a function. However, a student running both types of experiments will note that the exact shape of the hysteresis loops is very different: whereas the Ising model shows an almost rectangular shape (cf. Fig. 2), textbooks typically show an S-shaped form. However, even the usual graphs found in textbooks do not always depict reality correctly: the hysteresis loop has a small area (see Fig. 5). Thus, experiment and model do not agree completely. There are also deviations between model and theory: when taking the numerical derivative of the free energy, the curve looks almost (though not quite) like the magnetization plot; the derivations are best seen for small fields. This is likely because our entropy measurement is only an approximation and does not take long-range interactions into consideration.

This way, students learn that models are by their very nature incomplete and theories make approximations and can only predict reality within a certain error.

VI. A brief Introduction to Thermodynamics

Thermodynamics is the physics of temperature and heat. As a phenomenological science, it formulates the relations observed between physical observables. For example, for the ideal gas the product of pressure and volume is proportional to the temperature. Thermodynamics does not attempt to derive these relations from a microscopic theory.

Even though these relations are obvious to verify in an experiment, thermodynamics also formulates laws that are harder to verify experimentally. The most prominent example -the second law of thermodynamics first formulated by Clausius[14] - states the existence of a thermodynamic potential called the entropy, which cannot increase in closed systems. One of the consequences of this law is that thermodynamic processes, e.g. combustion engines transforming heat into mechanical work, must have a limited efficiency strictly below 1. Meaning it is impossible to convert heat energy into mechanical work without any loss[11] for temperatures T>0.
Since entropy is a rather abstract concept that cannot be measured directly, this law is -almost traditionally- hard to motivate to students. Some textbooks even joke that “students usually only believe this law because they wouldn’t otherwise pass their exam”.[4]

VII. Phenomenological Thermodynamics in the Remote Experiment

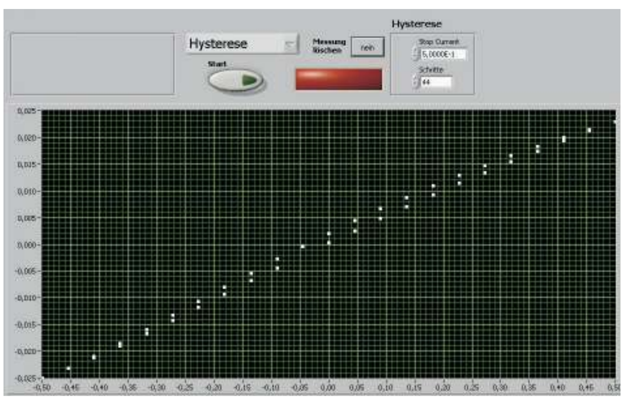

Figure 5. The hysteresis loop, as found by the remote experiment

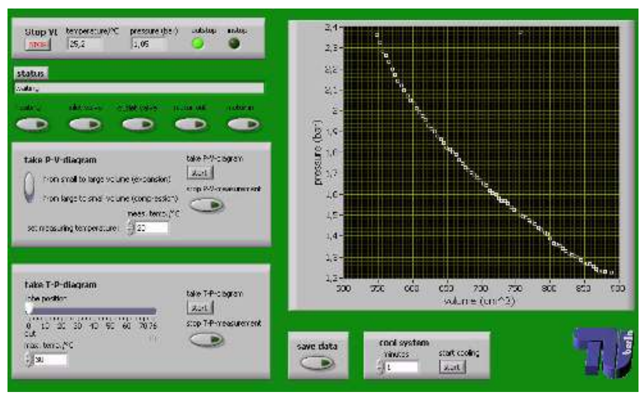

Figure 7. A pV diagram, as measured by the remote experiment

To demonstrate the classical gas laws, our remote experiment farm also includes an experiment on thermodynamics (see Fig 6). A motor controls the position of a piston in a glass cylinder containing air which temperature can be remotely adjusted by a heater. Sensors measure the pressure of the gas and its temperature. Their measurements are digitized and made available over the Internet. Given this setup, students can readily verify the classical laws of phenomenological thermodynamics, for example the Gay-Lussac relation between volume and temperature.

However, one can clearly go beyond this experiment: by controlling the heater and the piston, students can run the system in a thermodynamic cycle process. The amount of heat energy induced is known due to the characteristics of the heater and the amount of mechanical energy made available by a cycle can be computed from the area within the pV diagram[4] as measured, (see Fig. 7). Comparing the two readily presents the limited effectiveness of the process and demonstrates one of the consequences of the second law of thermodynamics.

VIII. Lattice Gases in the Virtual Laboratory

Lattice gases are simple, discrete models for ideal gases defined as cellular automata[9] and as such easily implementable in our virtual laboratory. Within HPP model used by our setup[2,3], the gas consists of elementary particles, atoms called in the following, which can only travel in four diagonal directions within two-dimensional space. Collisions with boundaries and between atoms preserve energy and momentum.

Unlike in remote experiments, we are now in a position where we know the microscopic state of the system exactly and able to measure the entropy. In a simple experiment, a student fills one corner of a simulated gas container with the lattice gas. If the simulation is run, the gas expands into all of the container and the entropy increases except for some small derivation (see Fig. 8).

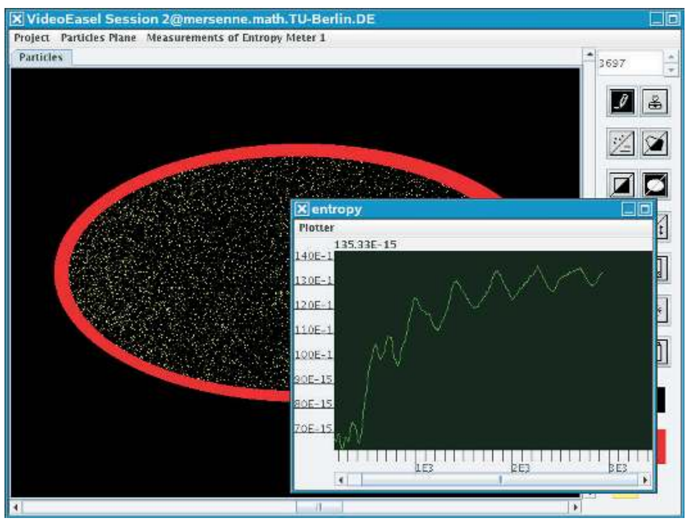

Figure 8. Final state after running the HPP gas for some time. Gas atoms in yellow, the boundary in red. In front plot of the entropy over time.

The monotonicity of the entropy looks even more surprising if we recapitulate that the elementary laws of the HPP gas are completely symmetric in time. The very same argument has been considered historically by Loschmidt as an objection against Boltzmann's H-Theorem[15,16] . Students are now, however, in a position where this objection can be discussed within an experiment, as our virtual laboratory provides means to invert all momenta. Quite as one might expect, gas atoms then move back to their initial positions and the entropy function decreases.

An experiment with such confusing outcome is well-suited to stimulate a vibrant discussion amongst our students. The resolution is now that the initial state of a gas running back into its container is extremely unlikely and with some guidance, students often come up with an experiment to justify this argument. After modifying the seemingly chaotic state by displacing a single atom by one pixel, we invert the moments of all gas atoms again and observe the entropy and the system behavior again. Even though the entropy starts to decrease for a short while, the system no longer comes close to the initial minimum and entropy begins to increase shortly after.

IX. Comparing Remote Experiments and Virtual Laboratories

It is worth noting that the pV looks again not very much like the idealized curves found in textbooks and is rather noisy. Good textbooks[4] will of course comment on such specialties. Similar differences often arise in real experiments, as we already found for the hysteresis experiment. They need to be discussed with the students and make up an important part of the education in physics, too.

On the other hand, we also find a tiny discrepancy between the phenomenologically formulated second law of thermodynamics and the corresponding outcome of the virtual experiment: it is not impossible that the entropy decreases, it is just that all odds are against it. Thus, the important lesson to be learned is that the second law makes a statement about the statistics of the system.

The complementary nature of remote experiments and virtual laboratories becomes even more apparent for the experiments on thermodynamics; while the remote experiment is targeted at the phenomenological side of thermodynamics, virtual laboratories allow to explore the statistical mathematical aspect of entropy. Thus, the dual nature of thermodynamical variables such as entropy — being a phenomenological quantity as well as a statistical one — can be explored and demonstrated.

X. Conclusion and Outlook

The accomplishment of experiments in eLearning scenarios touches many aspects — ranging from the actual quantification of a physical measurement over operating experience with real experimental setups to the examination of the corresponding theoretical model — of the learning process in the academic education of natural and engineering scientists. The combination of real experiments with virtual laboratories creates many benefits, the most important being the possibility for students to study a physical phenomenon throughout experiment, model and theory. We believe that the complementary nature of remote experiments and virtual laboratories stimulates the process of understanding in an outstanding matter, which is vital for the learning process in natural sciences.

Clearly, we still need to extend our experimental possibilities in both the remote as well the virtual laboratories. For example, we are not yet able to simulate a moving piston within our virtual laboratory as we would otherwise be able to provide an even closer simulation of the remote experiment and by that could measure pV diagrams in simulation.

Our work will also continue into another direction, namely in trying to perform experiments where virtual and real components interact, for example to compare their outcomes in a common plot within Maple, the mathematical algebra program. As both LabView and VideoEasel provide the necessary interfaces to export data, this goal seems to be in close reach.

Bibliography

1. E. Ising. Beitrag zur Theorie des Ferromagnetismus. Zeitschrift für Physik, 31:253–258, 1925.
2. J. Hardy, Y. Pomeau, and O. de Payssis. Time evolution of two-dimensional model system I: invariant states and time correlation functions. Journal of Mathematical Physics, 14:1746–1759, 1973.
3. J. Hardy, Y. Pomeau, and O. de Payssis. Molecular dynamics of a classical lattice gas: Transport properties and time correlation functions. Physics Review A, 13:1949–1961, 1976.
4. C. Gerthsen, H.O. Kneser, and H. Vogel. Physik. Springer, Berlin, 1977.
5. John D. Jackson. Classical Electrodynamics. John Wiley & Sons, New York, 1975.
6. L. Onsager. A two-dimensional model with an orderdisorder transformation. Phys. Rev., 65:117–149, 1944.
7. S. Jeschke, T. Richter, and R. Seiler. VideoEasel: Architecture of Virtual Laboratories on Mathematics and Natural Sciences. Proceedings of the 3rd International Conference on Multimedia and ICTs in Education, June 7-10, 2005, Caceres/Spain, Badajoz/Spain, June 2005. FORMATEX.
8. T. Richter. VideoEasel. http://www.math.tu-berlin.de/~thor/videoeasel .
9. T. Toffoli and N. Margolus. Cellular Automata Machines. MIT Press Cambridge, 1987.
10. N. Metropolis, A.W. Rosenbluth, M.N. Teller, and E. Teller. Equations of state calculations by fast computing machines. J. Chem. Phys, (21):1087–1091, 1953.
11. Friedrich Schlögl. Probability and Heat. Vieweg, Braunschweig, 1989.
12. National Instruments. Labview. http://www.ni.com/labview/ .
13. C. Thomsen, H. Scheel, and S. Morgner. Remote Experiments in Experimental Physics. Proceedings of the ISPRS E-Learning 2005, June 1-3, Potsdam/Germany, June 2005.
14. R. Clausius. Über die bewegende Kraft der Wärme und die Gesetze welche sich daraus für die Wärmelehre selbst ableiten lassen. Annalen der Physik und Chemie, 79:500–524, 1850.
15. J.L. Lebowitz. Boltzmanns entropy and times arrow. Physics Today, 46:32–38, 1993.
16. J. Loschmidt. volume 73 of Sitzungsber. Kais. Akad. Wiss. Wien, Math. Naturwiss., pages 128–142, 1876.