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C omp uter Simulations

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Recently the American Physical Society has established a new division "Computational Physics", in addition to its traditional divisions like Astrophysics, Nuclear Physics, Condensed Matter Physics, etc. This step is courageous as Computational Physics is by many colleagues still not accepted as a field in its own right. The traditional physicist finds his primary motivation in (often specialized) physical problems and considers a computational approach as one of many techniques which may lead to solutions. In contrast, the computational physicist specializes in numerical methods and tries to identify suitable physics problems. Often he or she supplements his or her approach then by other techniques. In practice the distinction is normally not as clear-cut as described. However, a substantial difference remains which allows one to clearly distinguish a computational from a traditional physicist. The question arises as to why one should choose to emphasize computational techniques to such an extent.

The development of mathematical calculus from the 18th century on allowed solutions of many physical problems with "unreasonable"

(Wigner) success. Here a typical mathematical solution provides a short cut. For instance in the case of the planetary two body problem, the solution of Newton's equations of motion gives the positions at all times. Instead of analytically solving the equations of motion one could construct it in small consecutive steps. Within the limit of a sufficiently small stepsize one would then obtain the correct result by adding up all the terms. The latter approach is typical for simulations. Until recently, before sufficient computer power had become easily accessible, it was fairly tedious to perform simulations. Still it would be impractical for the example at hand, since the exact solution is readily available. But nowadays the most important problems tend to be those for which exact solutions are either not available or more tedious to handle than a simulation. The ongoing computer revolution of the last decades may be expected to have a similarly relevant impact on science as the development of calculus in the past.

Simulational methods are very broad. I came to the Wissenschaftskolleg with the intention of looking out for applications outside physics, such as in economics, biology and social sciences. Basically there are two distinct types of simulation:

(a) deterministic simulations (as in our example)
(b) simulations based on randomness.

Deterministic simulations played a major role for modern developments in classical chaos theory. Examples, like a simulation of the Sinai billiard, were provided in various seminars of Hans Weidenmüller's "Chaos Group". Although partially overlapping, my own work did center more around simulations of type (b). Intrinsically based on chance, they go under the popular name "Monte Carlo Simulations". Results are obtained by statistical analysis of computer generated data. A particularly straightforward application is to simulate real statistical investigations, taking the needed probabilities from the empirical sample. In this way confidence limits of the empirical investigation can be "bootstrapped". Typically this is far simpler and more direct than applying standard statistical methods. At the Wissenschaftskolleg I had numerous discussions with Gideon Louw concerning the application of this method to biological field investigations and a joint paper might result. Another case I discussed with a few colleagues was motivated by the *Spiegel* rating of German universities, based on a poll from 10 637 students. The computational power of a Sun workstation at the Wissenschaftskolleg easily allows one to bootstrap the confidence levels of an investigation of this size.

For solving more complicated problems, the art within the Monte Carlo approach is to find suitable (best optimal) probabilistic weight factors to generate events. In statistical physics Monte Carlo simulations only became efficient after Metropolis et al. succeeded 1953 in incorporating

the Boltzmann weight in a feasible manner. From there on simulations of the so called "Canonical Ensemble" enjoyed steadily increasing popularity. Metropolis et al. performed their simulation on the Los Alamos "MANIAC". This was the supercomputer of their time. I re-programmed their application on the fastest Wissenschaftskolleg Sun workstation, and found that it runs by about $10^4 = 10000$ times faster than MANIAC. This explains why the method of Monte Carlo simulation is nowadays well practicable at non-specialized institutes. Present-day supercomputers run up to another factor 10^4 faster. Over forty years an acceleration by one order of magnitude (i. e., a factor of ten) was achieved approximately every five years. This ongoing rapid change constitutes the basis of the computer revolution.

In recent years I worked with various collaborators on generalizing the Metropolis approach. This led to a method known as "Multicanonical Monte Carlo Simulations". At the Wissenschaftskolleg work along this line was continued, resulting in five publications in respected peer-reviewed journals. The underlying Monte Carlo investigations and collaborations with internationally scattered colleagues were only feasible due to the good electronic facilities provided by Hans-Georg Lindenberg's EDV group.

To emphasize one paper, multicanonical simulation concepts inspired a general purpose "random-cost" optimization method which I published in *Nature.* Scientifically this is presumably the most interesting part of my work done at the Wissenschaftskolleg. Subsequently I began to test the method on the famous travelling salesman problem, which is to find the shortest closed path connecting N cities (N large). The generated data also attracted the interest of members of the chaos group, and various aspects are now being analyzed in collaboration with Oriol Bohigas and Thomas Seligman. This and other work, inspired here at the Wissenschaftskolleg, will certainly last well into the coming year.