John von Neumann Institute for Computing



Others

Peter Grassberger

published in

NIC Symposium 2006 ,
G. Münster, D. Wolf, M. Kremer (Editors),
John von Neumann Institute for Computing, Jülich,
NIC Series, Vol. **32**, ISBN 3-00-017351-X, pp. 323-324, 2006.

© 2006 by John von Neumann Institute for Computing
Permission to make digital or hard copies of portions of this work for personal or classroom use is granted provided that the copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. To copy otherwise requires prior specific permission by the publisher mentioned above.

http://www.fz-juelich.de/nic-series/volume32

Others

Peter Grassberger

Complex Systems Research Group
John von Neumann Institute for Computing
Research Centre Jülich, 52425 Jülich, Germany
E-mail: p.grassberger@fz-juelich.de

The contributions to this section are, as its title suggests, rather heterogeneous. Most are related to physics, at least by the fact that they were written by physicists who ventured out of the more narrowly defined discipline.

This is particularly true for the contribution of D. Stauffer, which is extreme in dealing on just eight pages with a number of problems taken from genetics, linguistics, social dynamics, and economics. Of course he cannot go into great depths, and of course the models are grossly simplified, so that they might look strange to "classical" researchers in these disciplines. But there is an increasing awareness that such simple and provocative models, usually agent-based and studied by simulations, can yield basic insights which cannot be obtained either from more realistic models or from mathematical models amenable to analytic treatment.

On the other extreme of particle based simulations is the contribution by P. Gibbon. Here the problem, the formation of plasmas by the impact of high intensity laser beams, is much less speculative and of direct technological relevance. The simulation uses state of the art methods, which find also applications in other fields such as astrophysics (stellar clusters), molecular biology (simulation of large macromolecules), and hydrodynamics. In all these fields one wants to simulate systems with millions of particles, often with long range interactions. Two main tricks help in reducing the formidable complexity of such problems: The introduction of 'mesoscopic' quasi-particles, and the approximation of potentials by the lowest terms of their multipole expansions. The contribution by Dr. Gibbon illustrates the difficulties in implementing them (together with other details), and the astonishing results obtainable thereby.

The contribution by E. Zienicke *et al.* is related to this in dealing also with plasma physics, but otherwise it is as far from it as it can be. The problem there is the transition to turbulence in magnetohydrodynamics, studied numerically by solving the relevant partial differential equations with a pseudospectral code. The chosen geometry, channel flow, is linearly stable in the regime where the transition to turbulence is found experimentally. This is similar to channel and pipe flow in ordinary hydrodynamics, where the last years have seen a break-through in understanding the mechanism for instability against *finite* perturbations from the laminar flow. Although the problem is much more difficult in the present case and requires the use of highest performance computers, it seems from the results obtained by Zienicke *et al.* that similar mechanisms are at work.

A rather different subject is dealt with in the contribution by G. Arnold *et al.*. As first pointed out by Feynman long ago, quantum mechanics has the potential of giving rise to extremely efficient computers. A general (pure) quantum mechanical state is a superposition of arbitrarily many eigenstates of any given operator, so that evolution of this state

is equivalent to the parallel evolution of arbitrarily many individual components. At this level, a computer based on this idea might seem just like a classical analog computer, but this is misleading because of the role played by the very structure of quantum mechanics. By now, not only algorithms for quantum computers exist which explicitly demonstrate their efficiency, but there are already first hardware prototypes – although using only very few qbits. The main difficulty in going to more qbits and thereby to real applications is decoherence. In order to understand its details, one has to make simulations (on classical computers!), which is what G. Arnold *et al.* do. Just because quantum computers are so efficient, simulating them on classical computers can be extremely time consuming and requires considerable resources, as illustrated well in their contribution.

Finally, with the last contribution by Bui Quang Minh *et al.*, we close the cycle by going from computer science back to genetics. The problem addressed there is the central one in molecular genetics, namely to find phylogenetic trees from DNA. With the complete genomes available for more and more species, one might think that it should become easier to reconstruct the tree of life. But all known methods are either inaccurate, or they require prohibitively much computational power (are NP-hard). Bui Quang Minh *et al.* first give a brief overview over these methods and present their own version. Then, they discuss in detail the implementation of their algorithm on the Jülich supercomputers, which makes up the main part of their paper. Although I personally would have preferred a more thorough discussion of the general problem, their treatment illustrates in an impressive way the achievements possible – and the efforts needed – when implementing state of the art algorithms on state of the art computers. Since this volume is edited by a supercomputer center and will be read mainly by its potential users, this might be exactly the information most useful for its readers.