Journal of Statistical Physics, Vol. 90, Nos. 5/6, 1998

Book Review: *The Art of Molecular Dynamics Simulation*

The Art of Molecular Dynamics Simulation. D. C. Rapaport, Cambridge University Press, Cambridge, 1995.

Molecular dynamics has been treated in many textbooks but I believe this is the first time we get a "hands on" version with all the paraphernalia needed for a practical guide to the subject. The author has prepared a well-proportioned and detailed work, written with enthusiasm and with numerous practical tips and illuminating examples. These range from a clear explanation of general ideas all the way to complete listings of computer programs. It is a must have for all the researchers working in this field, which fills the bill for practical use and as a standard reference.

The contents of the book are for the most part canonical. There is everything one might want to find in a recipe book on the subject of molecular dynamics simulations. In every case the emphasis is always on the "how to" aspect. The reader will find very few theoretical excursions that are not followed by detailed instructions for practical implementation, usually in the form of a (whole or part) computer program. The language of choice is C but the programs are written in such a way that a translation into Fortran, which is still the preferred choice of many workers in the field, should present no difficulty to those, who are unwilling to expand their language skills in computer programming. The numerous ready-to-use computer programs included in this book definitely set it apart from other textbooks on the subject. In a sense this is simply a cookbook of MD recipes.

The first five chapters (Introduction, Basic molecular dynamics, Simulating simple systems, Equilibrium properties of simple fluids, Dynamical properties of simple fluids) give the outlines of the basic landscape of the subject of molecular dynamics simulations. There is everything you already knew about MD but this time fully backed by listings of practical implementations and computer programs. They are preceded by detailed explanations of general principles and are, in general, easy to follow. Each

0022-4715/98/0300-1493$15.00/0

chapter ends with a "Further Work" section that could be used as homework problems in case you have to lecture on the subject. The explanations of the practical implementations are so detailed that you can actually take the book to your computer and simply start to program.

Other chapters concentrate on less canonical aspects of MD simulations (the definition of the word canonical of course will depend on the taste, background, and needs of the reader). There is a thorough introduction to the different ensembles in statistical mechanics and their implementation into MD stimulations. The author introduces the feedback and the constraint method to deal with controlled temperature and pressure ensembles, as well as in the case in which pressure is controlled by a variable region shape. What I missed in this class of problems is the introduction of the "contact theorem" in statistical mechanics which simplifies the evaluation of the stress tensor when one tries to calculate averaged interactions among groups of particles, parts of simulation systems or even bulk pressure itself. It has become indispensable in MC simulations of colloid interactions and I see no reason why this powerful method should not be used in MD simulations as well.

The chapters headed Rigid molecules, Flexible molecules, and Geometrically constrained molecules introduce all the necessary techniques for simulating rigid molecules (e.g., water) as well as polymers (e.g., alkane chains). The chapter headed Other interactions introduces the reader to the complications induced by long range potentials and non-pairwise additive potentials. Ewald sums feature prominently in this exposition but I believe they could be introduced more simply. Here again, practical examples more than compensate for this shortcoming. The dynamics of dipolar fluids is used as an example of the complications introduced into MD by long-range potentials. The opposite extreme, short range step potentials, are extensively analyzed in the following chapter. I also found particularly interesting the chapter on time dependent phenomena in which the author explains how the techniques of MD can be applied to the study of problems relating to thermal convection and obstructed hydrodynamic flow.

The concluding chapter introduces the reader to the use of supercomputers in MD simulations. It is probably only fair for a hands-on book like this one to end with a discussion of algorithm implementation for advanced computer architectures. An exposition, of course together with examples, of distributed MD computations and vector processing should satisfy hopeful advanced simulators, or at least give them solid directions for improving performance and accuracy of their computations.

I am sure this book will be a gem for everyone hoping to get hands-on experience with MD simulations. We can only hope that there will be

similar compilations of useful and practical recipes for other types of computer simulations, which are as satisfying as is this work.

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