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Book review

D.C. Rapaport, The Art of Molecular Dynamics Simulation, second ed., Cambridge University Press, ISBN 0-521-82568-7, 549 pages, hardback

The Art of Molecular Dynamics Simulation by D.C. Rapaport is one of many books introducing the rapidly maturing field of molecular dynamics (MD) simulations. MD simulations are used to analyze structural and dynamical properties of matter on an atomic scale and to provide (where possible) a link between microscopic detail and macroscopic behaviour. With both the development of advanced techniques and the rapid rise of computer power, MD simulations are nowadays increasingly used to study systems of biological relevance and as such could be useful to the readership of this journal. For anyone interested in applying these techniques, a good textbook introducing their possibilities and limitations is essential. In this review of the second edition of Rapaport's book, I will sketch its essential contents (in comparison to similar books on the topic) and discuss its suitability for potential audiences.

In his preface, Rapaport introduces the text as 'a combination of an introduction to MD for the beginner, and a cookbook and reference manual for the more experienced user'. Indeed, the book is built around full computer code listings of many algorithms and analysis tools that could serve as recipes for building one's own MD simulation suite. This is in contrast to many other textbooks in the field that introduce the material in a more conceptual manner and either use 'pseudo-code' as an illustration or no code at all. Rapaport does not start off with a few chapters on the theoretical (statistical mechanics) background of molecular simulations, but dives right into the subject, leaving the (active) reader with a first working MD code already by the end of Chapter 2. Throughout the book, this code is augmented in a modular fashion with more and more tools, the uses of which are illustrated with many different example systems. The philosophy of the author is to provide the reader with hands-on 'cooking' experience and expose him or her to various flavors along the way. For beginners working their way sequentially through the whole book, this would indeed work well. A disadvantage, however, is that many essential (and often related) pieces of knowledge are scattered throughout the text. This makes it hard to read (parts of) the book in a more browsing fashion and anyone trying to do so might miss out on important spices.

There are two reasons why this book seems less suitable to the experienced user than to the novice. First of all, the scattering of important information limits its function as a reference manual unless one just wants to use the available code. Second, and more importantly, the book does not provide a good account of more recent developments in the field. As far as the text is concerned, this second edition is hardly updated from the first edition. This is exemplified by the fact that of

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the 44 new references added, only four refer to papers published after 1999, and the chapter named 'the future' is almost literally the same as in the earlier edition. The French quote at the end of that chapter stating that the field is still in its infancy is hard to maintain almost ten years after the first edition. For these two reasons, I could only recommend the book to the beginning simulator who wants to write his own simulation code (which, for anyone entering the field, is a good thing to do), provided he finds more in-depth information on the state-of-the-art simulation practice on his system of interest from other sources. I will now discuss in some more detail the most essential aspects of the book.

Computer codes – As mentioned earlier, the book comes with full computer code listings, all available free of charge from the author's website. The programs have undergone a complete overhaul with respect to the first edition; they are all written in C and reflect the object-oriented nature of that language. Their conciseness and readability is superb and also easy to follow for people not familiar with C. Even when the material covered becomes increasingly complex (as for example in the quaternion scheme for rigid molecules or the Ewald summation scheme for treating long-range interactions), the codes remain very concise. This is accomplished by the extensive use of definition statements for many structures and macros that are used throughout the book. For reference, a complete list of these is given in one of the last chapters.

The author also included a chapter on algorithms for supercomputers, which is extremely helpful in modern times: The demand for simulations of large (bio)systems is ever increasing and available computer power currently rises faster by the numbers of processors per computer cluster than by single processor speed. Essential concepts that one needs to know when writing code for such architectures are well explained by Rapaport. Examples include the use of checkpointing, message passing schemes, and vector processing.

Theoretical basis – Unlike most other simulations textbooks, the book lacks a thorough introduction to the theoretical (statistical mechanics) background of simulations. Although this is a choice, and other sources can be consulted to fill that gap, it does occasionally seem to backfire. For instance, as there is no chapter to refer back to when introducing new theoretical concepts, most thermodynamic equations are merely posed, rather than derived. Sometimes, the concepts are explained rather vaguely (e.g. the introduction of periodic boundary conditions or the first mentioning of long-range interactions). This is a missed chance to provide the novice with the necessary toolkit to judge on his own which assumptions/approximations are important. Some statements may lead the inexperienced reader astray. For example, the book makes no clear distinction between thermodynamic temperature and its instantaneous 'estimator', the kinetic energy. It then goes on to introduce two types of thermostats: the Nosé-Hoover thermostat and one where the kinetic energy is rigorously constrained. While the latter is usually referred to as the 'isokinetic' thermostat, the book claims that both will lead to canonical averages. Clearly, all thermodynamic response functions that depend on fluctuations will be wrong in the isokinetic case (e.g., the heat capacity). This is a flaw that appears throughout the book. Other more minor things that suffer from lack of rigor are: Time-reversibility of the equations of motions is mentioned a few times in the book, but it remains unexplained why this is important. The book is also less than consistent with the number of degrees of freedom in the MD ensemble; once or twice three degrees of freedom are subtracted to account for momentum con-

servation, while in other cases this correction is dismissed as unimportant. Although such an approximation is indeed not severe for large systems, there is no reason why one should not be exact when one can at no extra cost.

Structure of the book – Overall, the book has a clear separation in chapters, organized by theme. The substructure inside a number of chapters, however, is much less transparent. There are quite a few examples where chapter sections deal with subjects that are not on the same level in thematical hierarchy. As an example, Chapter 4 deals with the equilibrium properties of fluids. After a section on structure, there is a separate section on packing studies (which is a subtheme), and then one on cluster analysis, which really belongs to packing studies as well. There are other chapters where results of example simulations are mentioned in different sections, even when there is yet another section called 'results' or 'measurements'. Most of the structural inconsistencies seem to have arisen where new sections were added with respect to the first edition. While all of the above do not really hamper the reading too much when the book is read from A to Z, it detracts from the use of the book as a reference manual.

Educational value – As already mentioned, the book is most suited for the beginner and should be really good for anyone wanting to learn to write one's first MD code. This is a very good educational experience for the novice, even if he or she will eventually make use of standard MD packages. Also good for the beginner is a quite elaborate discussion about the statistical relevance of measurements (including the concept of block averaging). This is not always valued enough by scientists working in the field, even though it is extremely important for translating simulation results (often on few and small systems over limited timescales) to the macroscopic world of experiments.

Apart from the above, there are a few topics covered by the book that generally are not covered by other simulation textbooks, and might thus be relevant to people who are especially interested in those themes. These include non-equilibrium systems, granular dynamics and cluster analysis.

On the negative side, the absence of a good introduction to more recent advanced simulation methods that was mentioned earlier is a drawback, also for the beginner. The most important omissions (especially for people interested in simulating biosystems) would be rare event techniques and/or coarse-graining approaches. The claim of the author that problems with system sizes and time scales are often not relevant since computer performance will outgrow the problems, will most likely not be agreed upon by the majority of present-day researchers.

In summary – The Art of Molecular Dynamics Simulation is an introductory textbook that gives a good feeling of what a well-written MD code should look like and – when worked through completely – gives a decent flavor of many tricks of the trade that one might encounter. As such, it would provide a good reference for a molecular simulation course aimed at people entering the field, provided they are guided by a teacher who fills in the background information that is missing in the book. The structure and readability of the book also lends itself for self study, but someone who aims to specialize in simulations would do well to follow up with one of the more advanced simulations textbooks to read up on the state-of-the-art in the field.

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